2005

Non-Cartesian distributed approximating functional

Troy Gerald Konshak
Iowa State University

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UMI®
Non-Cartesian distributed approximating functional

by

Troy Gerald Konshak

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Major: Physical Chemistry

Program of Study Committee:
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Iowa State University
Ames, Iowa
2005

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This is to certify that the doctoral dissertation of

Troy Gerald Konshak

has met the dissertation requirements of Iowa State University

Signature was redacted for privacy.

Committee Member

Signature was redacted for privacy.

Committee Member

Signature was redacted for privacy.

Committee Member

Signature was redacted for privacy.

Committee Member

Signature was redacted for privacy.

Major Professor

Signature was redacted for privacy.

For the Major Program
This work is dedicated to my wife and son who have proven that it is possible to have both a family and a Ph.D.
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### List of Acronyms

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<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIK</td>
<td>Approximating Identity Kernel</td>
</tr>
<tr>
<td>CMUS</td>
<td>Constrained Minimum Uncertainty State</td>
</tr>
<tr>
<td>CPDAF</td>
<td>Cartesian Product Distributed Approximating Functional</td>
</tr>
<tr>
<td>DAF</td>
<td>Distributed Approximating Functional</td>
</tr>
<tr>
<td>FEP</td>
<td>Free Evolution Propagator</td>
</tr>
<tr>
<td>FFT</td>
<td>Fast Fourier Transform</td>
</tr>
<tr>
<td>HTUP</td>
<td>Heisenberg Total Uncertainty Product</td>
</tr>
<tr>
<td>HUP</td>
<td>Heisenberg Uncertainty Product</td>
</tr>
<tr>
<td>MTUS</td>
<td>Minimum Total Uncertainty State</td>
</tr>
<tr>
<td>MUS</td>
<td>Minimum Uncertainty State</td>
</tr>
<tr>
<td>NCDAF</td>
<td>Non-Cartesian Distributed Approximating Functional</td>
</tr>
<tr>
<td>NCµ-Wavelet</td>
<td>Non-Cartesian Minimum Uncertainty Wavelet</td>
</tr>
<tr>
<td>RUP</td>
<td>Robertson Uncertainty Product</td>
</tr>
<tr>
<td>TDSE</td>
<td>Time Dependent Schrödinger Equation</td>
</tr>
</tbody>
</table>
Mathematical Notation

It will be assumed the reader is comfortable with the notation of undergraduate calculus [1], including elementary vector calculus [2][3], and Hilbert space methods used in quantum mechanics [4]. Discussed here is the shorthand employed in this thesis for handling quantities in arbitrary number of dimensions and coordinate systems\footnote{Note, attention will be restricted to Euclidean spaces.}.

The symbol

\[ \vec{a}^i, \]

will be used to indicate a vector quantity of \( D \) dimensions. A couple examples include using \( \vec{p}^i \) to indicate the momentum and using \( \vec{r}^i \) to indicate the location of the \( i^{th} \) sampled point. Components of a vector will be indicated with the same letter without the arrow and with a subscript. For example the components of \( \vec{p}^i \) will be written as \( p_1, p_2, \cdots, p_D \). An important example to note is, the components of \( \vec{r}^i \) will be written as \( r_{i,1}, r_{i,2}, \cdots, r_{i,D} \) where the reader needs to keep in mind that it is not a second rank tensor. It will be often be convenient to abbreviate the components of a vector that appear in the argument of a function by the vector symbol. For example,

\[ f(\vec{r}) = f(r_1, r_2, \cdots, r_D). \]

Two important vector operators that will be encountered often in this thesis are the gradient

\[ \nabla \vec{r} \]

and the Laplacian

\[ \nabla^2 \vec{r} . \]

It is important to note that this is in a coordinate system independent manner. For example, the
Laplacian could be expressed in $D$ dimensional rectangular coordinates as

$$\nabla^2 \tau = \sum_{i=1}^{D} \left( \frac{\partial}{\partial \tau_i} \right)^2,$$

or in hyperspherical coordinates [5] as

$$\nabla^2 \tau = \frac{1}{r^{D-1}} \frac{\partial}{\partial r} r^{D-1} \frac{\partial}{\partial r} - \frac{1}{r^2} \sum_{i>j}^{D} \left( r_i \frac{\partial}{\partial r_j} - r_j \frac{\partial}{\partial r_i} \right)^2,$$

where $r$ is the magnitude of $\tau^\bullet$.

Integrals over all components of a (real) vector will be symbolized by

$$\int_{\mathbb{R}^D} d\tau^\bullet f(r_1, r_2, \ldots, r_D),$$

where $\mathbb{R}^D$ symbolizes all of the real $D$ dimensional space. In rectangular coordinates for three dimensions this means

$$\int_{\mathbb{R}^3} d\tau^\bullet f(r_1, r_2, r_3) \equiv \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \ g(x, y, z),$$

and in spherical coordinates it is

$$\int_{\mathbb{R}^3} d\tau^\bullet f(r_1, r_2, r_3) \equiv \int_{0}^{2\pi} \sin \phi \ d\phi \int_{0}^{\pi} \ d\theta \int_{0}^{\infty} r^2 \ dr \ h(r, \theta, \phi),$$

where $g$ and $h$ are the function $f$ expressed in rectangular and spherical coordinates respectively. To illustrate the effect of a simple coordinate transformation consider the example where the variable $\tau^\bullet$ is related to $\tau^\bullet$ by

$$\tau^\bullet = \frac{1}{\sqrt{2\sigma}} (\tau^\bullet - \tau^{\bullet}_0).$$

In this case

$$dz_1 dz_2 \cdots dz_D = \left( \frac{1}{\sqrt{2\sigma}} \right)^D dr_1 dr_2 \cdots dr_D.$$
The result of the change of coordinates on the integral is

\[ \int_{\mathbb{R}^D} d\vec{r} \ f(\vec{z}_1, \vec{z}_2, \cdots \vec{z}_D) = \left( \frac{1}{\sqrt{2\pi}} \right)^D \int_{\mathbb{R}^D} d\vec{r} \ f(\vec{r}_1, \vec{r}_2, \cdots \vec{r}_D). \]

Operators will be denoted in bold font (e.g. \( \mathbf{H} \)) and vector operators will be distinguished with an arrow above (e.g. \( \vec{\mathbf{k}} \)). An important exception is the symbol \( \mathbf{I} \) that is reserved for the \( \sqrt{-1} \). It is also important not to confuse this symbol with \( \mathbf{I} \) which will be used to denote the identity operator. It will be necessary to introduce the symbol "\( \cdot \)" , which serves as an abstract inner (or dot) product; that is, for vector operators \( \vec{\mathbf{a}} \) and \( \vec{\mathbf{b}} \)

\[ \vec{\mathbf{a}} \cdot \vec{\mathbf{b}} = \sum_{i=1}^{D} a_i b_i. \]

It should be noted that \( \vec{\mathbf{a}} \cdot \vec{\mathbf{b}} \) does not in general equal \( \vec{\mathbf{b}} \cdot \vec{\mathbf{a}} \). The expression of this dot product in a representation is straightforward. For example, \( \vec{\mathbf{r}} \cdot \vec{\mathbf{r}} + \vec{\mathbf{k}} \cdot \vec{\mathbf{k}} \) corresponds to

\[ r^2 - \nabla^2 \]

in the position representation.
# List of Common Symbols

<table>
<thead>
<tr>
<th>symbol</th>
<th>meaning (unless otherwise noted)</th>
<th>additional info</th>
</tr>
</thead>
<tbody>
<tr>
<td>\cdot</td>
<td>dot product</td>
<td></td>
</tr>
<tr>
<td>\times</td>
<td>simple multiplication</td>
<td></td>
</tr>
<tr>
<td>[a, b]</td>
<td>commutator, ([a, b] = ab - ba)</td>
<td></td>
</tr>
<tr>
<td>[a, b]⁺</td>
<td>anti-commutator, ([a, b]⁺ = ab + ba)</td>
<td></td>
</tr>
<tr>
<td>[a; b]</td>
<td>dot commutator, ([a; b] = \overrightarrow{a} \cdot \overrightarrow{b} - \overrightarrow{b} \cdot \overrightarrow{a})</td>
<td>C2 p14</td>
</tr>
<tr>
<td>[a; b]⁺</td>
<td>dot anti-commutator, ([a; b]⁺ = \overrightarrow{a} \cdot \overrightarrow{b} + \overrightarrow{b} \cdot \overrightarrow{a})</td>
<td>C2 p16</td>
</tr>
<tr>
<td>\overrightarrow{a}</td>
<td>D-dimensional harmonic oscillator annihilation operator.</td>
<td>A3D</td>
</tr>
<tr>
<td>\overrightarrow{a}⁺</td>
<td>D-dimensional harmonic oscillator creation operator.</td>
<td>A3D</td>
</tr>
<tr>
<td>D</td>
<td>number of dimensions (degrees of freedom)</td>
<td></td>
</tr>
<tr>
<td>\delta(\overrightarrow{r'} - \overrightarrow{r})</td>
<td>D-dimensional Dirac delta functional</td>
<td></td>
</tr>
<tr>
<td>\delta</td>
<td>NCDAF (kernel) in the position representation</td>
<td></td>
</tr>
<tr>
<td>\delta_{CP}</td>
<td>CPDAF (kernel) in the position representation</td>
<td>C5 p204</td>
</tr>
<tr>
<td>\delta_{ij}</td>
<td>Kronecker delta</td>
<td></td>
</tr>
<tr>
<td>\delta_{ij}</td>
<td>(i, j)th element of the discrete NCDAF kernel</td>
<td></td>
</tr>
<tr>
<td>\Delta'</td>
<td>quadrature weight of the (d)th sampled point</td>
<td>C3 p140</td>
</tr>
<tr>
<td>\Delta or \Delta_{NC}</td>
<td>NCDAF in the momentum representation</td>
<td></td>
</tr>
<tr>
<td>\Delta_c</td>
<td>continuous NCDAF in the momentum representation</td>
<td></td>
</tr>
<tr>
<td>\Delta_d</td>
<td>discrete NCDAF in the momentum representation</td>
<td>C3 p159</td>
</tr>
<tr>
<td>\Delta_{CP}</td>
<td>CPDAF in the momentum representation</td>
<td>C5 p204</td>
</tr>
<tr>
<td>\nabla \overrightarrow{Z}</td>
<td>gradient (with respect to (\overrightarrow{z}))</td>
<td></td>
</tr>
<tr>
<td>\nabla^2 \overrightarrow{Z}</td>
<td>Laplacian (with respect to (\overrightarrow{z}))</td>
<td>p xi</td>
</tr>
<tr>
<td>\nabla^2 \overrightarrow{Z}</td>
<td>(\frac{1}{\sqrt{2\pi}} \nabla^2 \overrightarrow{r})</td>
<td></td>
</tr>
<tr>
<td>\nabla^2 \overrightarrow{Z}</td>
<td>(\frac{1}{2\sigma^2} \nabla^2 \overrightarrow{r})</td>
<td></td>
</tr>
<tr>
<td>\hbar</td>
<td>Planck's constant divided by (2\pi)</td>
<td></td>
</tr>
<tr>
<td>symbol</td>
<td>meaning (unless otherwise noted)</td>
<td>additional info</td>
</tr>
<tr>
<td>--------</td>
<td>----------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>$i$</td>
<td>$\sqrt{-1}$</td>
<td></td>
</tr>
<tr>
<td>$I$</td>
<td>identity operator</td>
<td></td>
</tr>
<tr>
<td>$\vec{k}$</td>
<td>$\frac{1}{\hbar} \vec{p}$, momentum scaled by $\hbar$, aka the wavevector</td>
<td></td>
</tr>
<tr>
<td>$\vec{k}$</td>
<td>momentum operator scaled by $\hbar$ (abstract form)</td>
<td></td>
</tr>
<tr>
<td>$\vec{K}$</td>
<td>$\vec{k} - \vec{k}_0$, where $\vec{k}$ is the dependent variable and $\vec{k}_0$ is a reference point</td>
<td></td>
</tr>
<tr>
<td>$\vec{K}$</td>
<td>$\vec{k} - \langle \vec{k} \rangle$, (abstract) operator form</td>
<td></td>
</tr>
<tr>
<td>$\zeta$</td>
<td>$\frac{1}{\sqrt{2}} \sigma K$</td>
<td></td>
</tr>
<tr>
<td>$\zeta$</td>
<td>$\frac{1}{\sqrt{2}} \sigma K$, (abstract) operator form</td>
<td></td>
</tr>
<tr>
<td>$L_n^m(a)$</td>
<td>associated Laguerre function (polynomial)</td>
<td>C3 p75</td>
</tr>
<tr>
<td>$L_n^{D/2-1}(z^2)$</td>
<td>$l = 0$ NCDAF polynomial</td>
<td>C3 p77</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>NC$\mu$-Wavelet lowering operator.</td>
<td>S3.3</td>
</tr>
<tr>
<td>$\Lambda_n$</td>
<td>NCDAF free evolution propagator polynomial</td>
<td>C7 p278</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>NC$\mu$-Wavelet lowering operator for $n \to n - 1$ with fixed $l$</td>
<td>S3.3</td>
</tr>
<tr>
<td>$M$ or $M_{NC}$</td>
<td>NCDAF degree parameter</td>
<td></td>
</tr>
<tr>
<td>$M_{CP}$</td>
<td>CPDAF degree parameter</td>
<td>C5 p203</td>
</tr>
<tr>
<td>$\sigma$ or $\sigma_{NC}$</td>
<td>NCDAF width parameter</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{CP}$</td>
<td>CPDAF width parameter</td>
<td>C5 p203</td>
</tr>
<tr>
<td>$\delta$</td>
<td>NCDAF width parameter scaled by grid spacing</td>
<td>A4C</td>
</tr>
<tr>
<td>$\vec{r}$</td>
<td>position</td>
<td></td>
</tr>
<tr>
<td>$\vec{r}$</td>
<td>position operator (abstract form)</td>
<td></td>
</tr>
<tr>
<td>$\vec{R}$</td>
<td>$\vec{r} - \vec{r}_0$, where $\vec{r}$ is the dependent variable and $\vec{r}_0$ is a reference point</td>
<td></td>
</tr>
<tr>
<td>$\vec{R}$</td>
<td>$\vec{r} - \langle \vec{r} \rangle$, (abstract) operator form</td>
<td></td>
</tr>
<tr>
<td>symbol</td>
<td>meaning (unless otherwise noted)</td>
<td>additional info</td>
</tr>
<tr>
<td>------------</td>
<td>-------------------------------------------------------------------------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>$R_{DAF}$</td>
<td>half bandwidth of the NCDAF kernel</td>
<td>C3 p211</td>
</tr>
<tr>
<td>$\overline{\rho}$</td>
<td>NC$\mu$-Wavelet raising operator.</td>
<td>S3.3</td>
</tr>
<tr>
<td>P (rho)</td>
<td>NC$\mu$-Wavelet raising operator for $n \rightarrow n + 1$ with fixed $l$</td>
<td>S3.3</td>
</tr>
<tr>
<td>$U^2$</td>
<td>square of the uncertainty product</td>
<td>C2 p12</td>
</tr>
<tr>
<td>$U_n^2$</td>
<td>square of the $n^{th}$ constrained uncertainty product</td>
<td>C2 p30</td>
</tr>
<tr>
<td>$W_{DAF}$</td>
<td>$R_{DAF}/\Delta$, where $\Delta$ is the spacing between points</td>
<td>C3 p142</td>
</tr>
<tr>
<td>$\overline{\Psi}$</td>
<td>$\sqrt{2\sigma} \vec{k}$, (abstract) operator form</td>
<td>S3.3</td>
</tr>
<tr>
<td>$\overline{\Psi}$</td>
<td>$\sqrt{2\sigma} \vec{k}$, (abstract) operator form</td>
<td>S3.3</td>
</tr>
<tr>
<td>$\overline{Z}$</td>
<td>$\frac{1}{\sqrt{2\sigma}} \vec{R}$, (abstract) operator form</td>
<td>S3.3</td>
</tr>
<tr>
<td>$\overline{Z}$</td>
<td>$\frac{1}{\sqrt{2\sigma}} \vec{R}$, (abstract) operator form</td>
<td>S3.3</td>
</tr>
<tr>
<td>$\overline{Z} L_n^{D/2}(Z^2)$</td>
<td>$l = 1$ NCDAF polynomial</td>
<td>C3 p77</td>
</tr>
<tr>
<td>$[\overline{Z}]^t$</td>
<td>$t^{th}$ rank irreducible Cartesian tensor generated from $\overline{Z}$</td>
<td>C3 p77</td>
</tr>
<tr>
<td>$[\overline{Z}]^t L_n^{D/2-1+i}(Z^2)$</td>
<td>$(n, l)^{th}$ NCDAF polynomial</td>
<td>C3 p77</td>
</tr>
<tr>
<td>$\xi$</td>
<td>$\frac{1}{2} \sigma^2 \vec{K}^2$</td>
<td></td>
</tr>
<tr>
<td>$\xi$</td>
<td>$\frac{1}{2} \sigma^2 \overline{\vec{K} \cdot \vec{K}}$, (abstract) operator form</td>
<td></td>
</tr>
</tbody>
</table>
Abstract

Presented in this work is the Non-Cartesian Distributed Approximation Functional (NCDAF). It is a multi-dimensional generalization of the (one-dimensional) Hermite DAF that is non-separable and isotropic. Demonstrated here is an approximation method based on the NCDAF that can construct a continuous approximation of a function and derivatives from a discrete sampling of points. Under appropriate choice of conditions this approximation is free from artifacts originating from 1) the sampling scheme, and 2) the orientation of the sampled data. The NCDAF is also viewed as a compromise between the minimum uncertainty state (i.e. Gaussian) and the ideal filter. The NCDAF (kernel) is shown 1) to have a very small uncertainty product, 2) to be infinitely smooth, 3) to possess the same set of invariances as the minimum uncertainty state, 4) to propagates in convenient closed form under quantum mechanical free propagation, and 5) can be made arbitrarily close to the ideal filter.
1 Introduction

Digital informatics has truly revolutionized science and technology. Experimental data for phenomena with continuous variables is now dominantly collected, stored, and analyzed by discrete sampling. This includes examples such as seismic data [6][7], x-ray images [8][9], and fingerprints [10] that are strongly associated with analog representations. Digital informatics has also spawned totally new areas of research such as computer vision [11][12]. Consumer technology has even been revolutionized by the overwhelming dominance of digital photography, movies, and music.

Discrete grid methods are also useful in theoretical studies. Potential energy surfaces are generated as discrete values in configuration space of nuclear distances and angles [13]-[15]. Solutions to partial differential equations are also conveniently found using grid methods [16, p818-880]-[18]. Similarly, grid methods are useful for solving integral equations [16, p779-817][19, p779-817].

The theoretical concept behind grid methods is the Shannon-Nyquist theorem [20][21]. It states that a function composed of a finite, but not necessarily discrete, range of frequencies can be exactly represented by a discrete sampling. A corollary of this theorem is that for a given (frequency) band-limited function there is a maximum sampling rate, known as the Nyquist frequency, above which no further information about the function is obtained\(^2\). What makes the theorem of practical utility is that the essential features of many phenomena can be considered to be band-limited. Though this is an approximation, it is often a very accurate one.

There are a number of goals that any method for analyzing data represented discretely on a grid should strive to meet. An important one is that the method should accurately approximate the function underlying the phenomenon producing the data between sampled points. This is the goal of function approximation methods [16, p99-122]. It is also desirable that there be no perceivable difference between the approximation on and off the grid points. Approximations with this property are known as well-tempered [22]. This is part of the broader goal that the approximation should not contain any artificial

\(^2\)It should be mentioned that if the data contains noise then sampling above this maximum rate (oversampling) can be useful for reducing the noise.
structure induced by the approximating method. An example application where this is important is computer vision. In this case, the aim is to see the world as naturally as possible. Another goal is that linear operators, such as derivatives, should be represented accurately. This is very important for solving partial differential equations using grid methods and characterizing special points on potential surfaces. A challenging goal for approximation methods is to approximate functions within large gaps of data. This is particularly difficult when the gap is significantly larger than the Nyquist wavelength (i.e. $\lambda_{\text{Nyquist}} = \pi/f_{\text{Nyquist}}$) of the data. In such situations the missing data can contain several oscillations. Analysis methods should also generalize to multiple dimensions without preferred directions or orientations. The reason is that these biases can lead to undesirable effects [23]. For example, the commonly employed generalization using Cartesian products of one-dimensional functions can result in approximations with artificial rectangular structure. An important component of all these goals is the requirement of computational efficiency.

One mathematical structure for an approximation method that meets these goals is the Distributed Approximating Functional (DAF) [24]-[26]. Unlike many other methods, such as polynomial [16, p102-104][28] and splines methods [16, p99-122][27][29], the DAF approximation does not contain any special points. That is, the requirement that the approximation be exact on the sampled points is relaxed in favor of a well-tempered approximation. As a result the approximation on and off the grid points is of the same order of accuracy. This has been useful in providing accurate representations of potential energy surfaces from discrete samples [30]-[33]. The DAF first derivative approximation can also be made to be within the same order of accuracy as the function approximation. The DAF second derivative approximation, likewise, is within an order of accuracy of the previous first derivative approximation. Higher order DAF derivative approximations show this general trend. This has lead to highly accurate and robust solutions to many challenging partial differential equations [34]-[43]. The high accuracy of the DAF approximation is accompanied by properties that make it computationally efficient. The discrete DAF representation of many important operators (e.g. the identity, the gradient, the Laplacian and combinations thereof) have a couple of major advantages: 1) their representation can be relatively
sparse in the position domain, and 2) for uniformly distributed grids, their representation is toeplitz [16, p82-89][44] (i.e. the elements, $A_{ij}$, depend only on the difference of $i-j$). The first is related to the diagonal dominance and Gaussian decay away from diagonal. This is highly advantageous, for example computing the application of the operator or finding its eigenvalues. The second, the toeplitz structure implies there are only a small number of distinct matrix elements. Consequently, the whole matrix can be generated very quickly with relatively small storage requirements. The DAF approximation is a convolution meaning that it is a simple multiplication in the Fourier space (i.e. momentum domain).

Presented in this thesis is the multi-dimensional generalization of the DAF known as the Non-Cartesian Distributed Approximating Functional (NCDAF) [45]. As the name suggests, it is not a simple Cartesian product of the one-dimensional functions. This generalization is isotropic, leading to no bias towards any particular orientation of axis. As will be demonstrated, the NCDAF retains all the advantages of its one-dimensional counterpart. This includes the important property of not introducing an artificial structure into the approximation of the data.

An important concept in any area where information possesses a Fourier transform structure is the uncertainty principle [46][47][48]. The principle states that there is a lower limit on the accuracy of the simultaneous measurement of conjugate observables. Example conjugate observables include: the position and momentum of a (quantum) particle, the time and energy of a scattering event, and the frequency and time in a signal. To understand the principle it is useful to review the Heisenberg-Bohr microscope. In W. Heisenberg's The Physical Principles of the Quantum Theory [47], he describes the system as follows:

...Let the particle be moving at such a distance from the microscope that the cone of rays scattered from it through the objective has an angular opening $\epsilon$. If $\lambda$ is the wave-length of
the light illuminating it, then the uncertainty in the measurement of the $x$-co-ordinate,

\[
\Delta x = \frac{\lambda}{\sin \epsilon}.
\]

But, for any measurement to be possible at least one photon must be scattered from the electron and pass through the microscope to the eye of the observer. From this photon the electron receives a Compton recoil of magnitude $\frac{h}{\lambda}$ [where $h$ is Planck's constant]. The recoil cannot be exactly known, since the direction of the scattered photon is undetermined within the bundle of rays entering the microscope. Thus there is an uncertainty of the recoil in the $x$-direction of amount

\[
\Delta p_x \sim \frac{h}{\lambda} \sin \epsilon,
\]

and it follows that for the motion after the experiment

\[
\Delta x \Delta p_x \sim h
\]

[47, p21].

An important aspect of this example to note is the inverse relationship between the uncertainty in position and momentum. That is, the uncertainty in position can be decreased by using a smaller wave-
length of light, but the uncertainty in momentum (which is inversely proportional to the wavelength) will increase by the same factor. In the limit of where the position is exactly known the momentum uncertainty will be infinite. For an elementary discussion of several other examples the reader is referred to reference [49]. Although most often associated with quantum mechanics, uncertainty principles are pervasive in a wide range of fields. As an example in signal processing, consider the function depicted in the following diagram:

Clearly the function is more oscillatory, compared to the rest of the function, around points \( t = -5 \) and 6.5. By counting the number of oscillations within a conveniently small time range around these two features, a frequency range of about 1.15 to 1.25 can be associated with the features. As is well-known, it is not possible to assign a precise frequency to a specific time point in the signal (e.g. at \(-5\) or 6.5). This situation is completely analogous to the position-momentum uncertainty relationship in quantum mechanics. Other fields where the uncertainty principle is pervasive include radar and remote sensing, optics, filters, pattern recognition, and data compression. In mathematical terms, any analysis method that is fundamentally based on Fourier analysis is subject to an uncertainty principle.

The quantity,

\[ \Delta x \Delta p_x , \]
is an example of the Heisenberg uncertainty product (HUP). Although a HUP exists for any two conjugate observables, attention in this discussion will be limited to the above example. In addition to giving the limitation on the accuracy of simultaneous measurements of conjugate observables, the HUP defines the wavefunction for which the minimum value of uncertainty product is realized. These wavefunctions are known as minimum uncertainty states (MUS) and possess the important property of being optimally localized in phase space (position-momentum product space). Such states are of importance to a wide range of fields such as semiclassical physics [50] and quantum computing [51][52]. MUS also possess a number of other desirable properties that make them useful in Fourier based analysis methods. The most important is that they allow data to be decomposed into parts with narrow ranges of both position and momentum (or time and frequency, etc.).

It has been shown that Distributed Approximating Functionals are closely related to MUSs [53][54][55]. The connection is made by interpreting DAFs as constrained minimizers of the HUP. An important result is that DAFs provide a systematic way to improve the resolution of one of the observables, at the expense of a minimal increase in uncertainty of the conjugate observable and the uncertainty product. DAFs have also been shown to share many desirable properties of MUSs.

Like the special case of one dimension, the NCDAF can be derived using a constrained minimization of an uncertainty product. The appropriate multidimensional uncertainty product will be shown to be for the system’s total momentum and conjugate (total) position. This "Heisenberg total uncertainty product" leads to constrained minimum uncertainty states with the desirable isotropic property. The NCDAF will be seen to be a compromise between the MUS and the (isotropic) ideal filter.

An important application of the DAF is the approximation of propagators [34][56]-[63]. Propagators, as the name suggests, are operators that propagate a state over a (real or imaginary) time interval. One of the most important propagators is the quantum mechanical free evolution propagator [64]. Since many propagators can be approximated with split operator techniques [65][66][67] involving the free evolution propagator, its approximation is especially important. The usefulness of the DAF to approximate the action of propagators can be traced to the fact that the action of the free evolution
propagator on the DAF approximation is known in a convenient closed form. Like many of the other uses of the DAF, the approximation of propagators can be generalized to the NCDAF case.

This thesis is organized as follows. In the second chapter, the relation of the NCDAF to the uncertainty principle will be established. Some basic properties of the NCDAF are also discussed. In the third chapter, convenient polynomial expressions for the NCDAF and its derivatives are derived. A number of properties of, and relationships among, the NCDAF polynomials are detailed. These will be important for deriving efficient and accurate implementations of the NCDAF in numerical applications. The second half of chapter three is devoted to examining the Non-Cartesian Minimum Uncertainty Wavelets (NCμ-Wavelets) that are the fundamental components of the NCDAF. The fourth chapter explores many important numerical properties of the NCDAF approximation of functions and derivatives. The numerical foundation of NCDAF will also be established. The isotropic nature of the NCDAF approximation to functions will be discussed in the fifth chapter. This will be done by comparing the NCDAF to the alternative Cartesian Product DAF (CPDAF) approach to function approximations. The approximation of functions within large gaps of data is discussed in chapter six. In chapter seven, the NCDAF representation of the quantum mechanical free evolution propagator is developed. Chapter eight will summarize the important findings of this thesis. Suggestions for future research and applications are also discussed.
2 Non-Cartesian Distributed Approximating Functionals as Constrained Minimum States of the Heisenberg Total Uncertainty Product

In signal (image, and higher dimensional data) processing the data often needs to be differentiated, integrated, smoothed, interpolated, extrapolated, noise reduced, or Fourier analyzed. Various combinations of these operations are vital to applications such as radar and other remote sensing [68], feature extraction and pattern recognition [69], compression [71], and solutions to partial differential equations [70]. All of the above operations can be formulated in terms of filters [72]. The basic\footnote{i.e. linear and non-recursive} filter expression is

\[ g(\vec{r}) = \int_{\mathbb{R}^D} d\vec{r}' \phi(\vec{r}' - \vec{r}) f(\vec{r}') \, , \]  

where \( f \) is the input function, \( \phi \) is the filter, and \( g \) is the output function. It is important to note that this expression is a convolution [2] which means that in the Fourier domain the corresponding expression is a simple multiplication,

\[ G(\vec{k}) = \Phi(\vec{k}) F(\vec{k}) \, , \]  

where \( G, \Phi, \) and \( F \) are the Fourier transforms of \( g, \phi, \) and \( f \) respectively.

Many of the desirable properties of filters are embodied in two archetypes known as the ideal and Gaussian filters. The ideal or 'square' filter refers to a window in momentum space that allows a range of momenta (or frequencies) to pass through unaltered with all others totally blocked. This is a useful property for applications requiring a clean partitioning of frequencies such as noise reduction [73] and multi-resolution analysis [74]. A desirable property of the Gaussian filter is that is near local in phase space, i.e. signal-frequency product space. As a matter of fact, the Gaussian filter has the smallest
possible localization permitted by the *Heisenberg uncertainty principle* [4, p286-289]. This is important to any Fourier based analysis method. Another desirable property of the Gaussian filter is its infinite smoothness. That is, the Gaussian filter is differentiable to all orders everywhere. This is obviously important to data smoothing (removing discontinuities) and for differentiating.

Of particular interest is how the above desirable properties can be incorporated into a single filter. This is because the key properties of the ideal and the Gaussian filter are incompatible. The conflicts are 1) the Gaussian attenuates the entire momentum spectrum (except at the origin), 2) the uncertainty product for the ideal filter is infinite, and 3) the ideal filter is not smooth to any order. Introduced in this chapter is the Non-Cartesian Distributed Approximating Functional (NCDAF) [45], which provides a good compromise between these conflicts. This was first realized in the Physical Review letter [53] and expanded in papers [54][55][75]. The compromise is realized by employing a constrained minimization of the uncertainty product. The resulting NCDAF function is infinitely smooth, highly localized in phase space, and provides an arbitrarily close reproduction of the frequency spectra over an adjustable range.

Another desirable property for filters in multi-dimensions is isotropy. This prevents an artificial bias from being induced into the analysis of the data, which can be troublesome in applications such as compression and image analysis [23]. To incorporate this property it will be necessary to formulate an uncertainty product that treats the degrees of freedom collectively. Besides leading to an isotropic constrained minimum, the resulting NCDAF is non-separable and independent of the choice of coordinate system [45].

In the first section, the form of the Heisenberg uncertainty product that will lead to an isotropic constrained minimum is discussed. The minimum uncertainty state of this Heisenberg uncertainty product is derived in the next section. A number of the minimum uncertainty state's properties are also discussed in the second section. In the third section, the constrained minimization of the Heisenberg uncertainty product is carried out. A few general properties of the constrained minimum are then discussed with a couple of examples given. The fourth section identifies the case that is the NCDAF.
Lastly, a few basic properties of the NCDAF are discussed.

### 2.1 Heisenberg Total Uncertainty Product

Perhaps the most distinctive characteristic of quantum mechanics is the limitation it imposes on measurements. The origin of this phenomenon can be traced to the fact that observables are represented by operators in Hilbert space [76]. The uncertainty in the measurement of an observable is thus formulated as the dispersion, or root-mean-square deviation, of its corresponding operator; symbolically,

\[
(\Delta a) = \sqrt{\langle \psi | (a - \langle a \rangle)^2 | \psi \rangle / \langle \psi | \psi \rangle},
\]

(2.3)

where \( \langle a \rangle \) is the expectation value of the observable \( a \), and \( | \psi \rangle \) is the Hilbert space vector that represents the state of the system in which the measurement is made. An interesting situation arises when the simultaneous measurement of another observable is attempted. This is most clearly understood when the second observable is the conjugate observable to the first. Conjugate observable pairs are ones defined by

\[
[a, b] = \pm i\hbar I,
\]

(2.4)

where \( [a, b] = ab - ba \) is the commutator, the + or − is determined by the convention used in the definition of the observables, \( I = \sqrt{-1} \), \( \hbar \) is Planck's constant divided by \( 2\pi \), and \( I \) is the identity operator. The consequence of this is that the uncertainty for simultaneous measurement of the conjugate operators is

\[
(\Delta a) (\Delta b) \geq \frac{1}{2} \sqrt{\left| \langle \psi | [a, b]_+ | \psi \rangle / \langle \psi | \psi \rangle \right|^2 + \hbar^2},
\]

(2.5)

where \( [a, b]_+ = ab + ba \) is the anti-commutator. This uncertainty product thus has a lower bound, specifically

\[
(\Delta a) (\Delta b) \geq \frac{1}{2} \hbar,
\]

(2.6)
which is the famous Heisenberg uncertainty principle [47]. Although this expression is valid for any two conjugate observables, attention will be restricted to the example case where they are position and momentum,

\[ (\Delta x) (\Delta p) \geq \frac{1}{2} \hbar, \]  

(2.7)

with right hand side representing the minimum phase space area in which a state can be measured.

The uncertainty product for a system of more than one degree of freedom can be formulated a few different ways. The standard expression for the multi-dimensional Heisenberg uncertainty product [4][77] is

\[ (\Delta x_i) (\Delta p_j) \geq \frac{1}{2} \delta_{ij} \hbar, \]  

(2.8)

where \( \delta_{ij} \) is the identity tensor. It is important to note that this expression is a second rank tensor but it transforms as a scalar. The expression can be reduced to a number by either 1) taking the trace, as shown by

\[ (\Delta x_1) (\Delta p_1) + (\Delta x_2) (\Delta p_2) + \cdots + (\Delta x_D) (\Delta p_D) \geq \frac{D}{2} \hbar, \]  

(2.9)

or 2) taking the determinant, as shown by

\[ |(\Delta x_i) (\Delta p_j)| \geq \left(\frac{1}{2} \hbar\right)^D, \]  

(2.10)

where \( D \) is the number of dimensions. The first approach is clearly the sum of 1D Heisenberg uncertainty products. The second can be simplified further [78] to obtain

\[ (\Delta x_1) (\Delta p_1) (\Delta x_2) (\Delta p_2) \cdots (\Delta x_D) (\Delta p_D) \geq \left(\frac{1}{2} \hbar\right)^D, \]  

(2.11)

which is the product of 1D Heisenberg uncertainty products. It should be noted that this second approach is a special case of the Robertson uncertainty product (RUP). For details on the RUP the reader is referred to reference [78]. It is important to note that in either approach the degrees of
freedom are treated independently. Alternatively one may wish to consider the uncertainty product for the overall system. This corresponds to the simultaneous measurement of the magnitude of total momentum,

\[ p_T = \sqrt{p_1^2 + p_2^2 + \cdots + p_D^2}, \tag{2.12} \]

and its conjugate magnitude of total position,

\[ r_T = \sqrt{x_1^2 + x_2^2 + \cdots + x_D^2}. \tag{2.13} \]

It should be clear that these quantities are the magnitude of the momentum and position vectors, \( \vec{p} \) and \( \vec{r} \) respectively. This type of measurement is thus measuring the length of the vectors. The corresponding uncertainty product can therefore be expressed as

\[ (\Delta |\vec{r}|) (\Delta |\vec{p}|) = U, \tag{2.14} \]

which will be referred to as the Heisenberg Total Uncertainty Product (HTUP). To find the explicit expression for the HTUP it will be necessary to derive it from fundamental principles.

First, the operator expression for the total momentum and conjugate position operators needs to be determined. Start by considering the position and conjugate momentum operators for an arbitrary number of degrees of freedom, symbolized by \( \vec{r} \) and \( \vec{k} \) respectively (where \( \vec{k} \) the wavevector, which is \( \vec{p} \) scaled by \( \hbar \) so it has units of inverse length). It should be noted that these are vector operators meaning that

\[
\begin{array}{c|cc}
\text{r representation} & \text{k representation} \\
\hline
\vec{r} & \vec{r} & +i\vec{\nabla}x \\
\vec{k} & -i\vec{\nabla}r & \vec{k} \\
\end{array}
, \tag{2.15}
\]

where the arrow indicates a vector quantity of \( D \) dimensions and \( \vec{\nabla} \) is the gradient. It is convenient to
use operators that are shifted by their expectation values,

\[
\begin{align*}
\overrightarrow{R} &= \overrightarrow{r} - \langle \overrightarrow{r} \rangle = \overrightarrow{r} - \overrightarrow{r}_0 \quad (2.16a) \\
\overrightarrow{K} &= \overrightarrow{k} - \langle \overrightarrow{k} \rangle = \overrightarrow{k} - \overrightarrow{k}_0 , \quad (2.16b)
\end{align*}
\]

such that the new operators have vanishing expectation values, \( \langle \overrightarrow{R} \rangle = 0 \) and \( \langle \overrightarrow{K} \rangle = 0 \). The square of total momentum and conjugate position are thus given by

\[
\begin{align*}
\overrightarrow{K} \cdot \overrightarrow{K} \quad (2.17a) \\
\overrightarrow{R} \cdot \overrightarrow{R} , \quad (2.17b)
\end{align*}
\]

where the dot (\( \cdot \)) indicates the scalar product of these vector operators.

A useful commutator relationship can now be derived (by generalizing the procedures of [77, p299-301] and [79, p260-261]). Consider the action of \( \overrightarrow{K} \cdot \overrightarrow{R} \) on an arbitrary state in the position representation,

\[
\begin{align*}
\overrightarrow{K} \cdot \overrightarrow{R} \psi &= -i \overleftarrow{\nabla}_R \cdot \{ \overrightarrow{R} \psi \} \quad (2.18a) \\
&= -i \left( \{ \overleftarrow{\nabla}_R \cdot \overrightarrow{R} \} \psi + \overrightarrow{R} \cdot \{ \overleftarrow{\nabla}_R \psi \} \right) \quad (2.18b) \\
&= \left( -i \delta I + \overrightarrow{R} \cdot \overrightarrow{K} \right) \psi . \quad (2.18c)
\end{align*}
\]

The result is the commutator-like expression,

\[
\overrightarrow{K} \cdot \overrightarrow{R} - \overrightarrow{R} \cdot \overrightarrow{K} = i \delta I . \quad (2.19)
\]
which will be called the dot product commutator and symbolized by

\[ [\vec{R}, \vec{K}] = i\Omega, \]  

(2.20)

with the semi-colon (\( ; \)) distinguishing it from the ordinary commutator.

Another concept that needs to be established is the validity of Schwarz inequality [4, p 165][80] to the case of dotted operators. Consider the operator\(^2\)

\[ Q = I - \frac{\vec{B} |\phi\rangle \langle \phi| \vec{B}}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle}, \]  

(2.21)

where \( \vec{B} \) is a Hermitian operator, \( I \) is the identity operator, and \( |\phi\rangle \) corresponds to a normalizable state. When dotted into itself,

\[ Q \cdot Q = \left( I - \frac{\vec{B} |\phi\rangle \langle \phi| \vec{B}}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle} \right) \cdot \left( I - \frac{\vec{B} |\phi\rangle \langle \phi| \vec{B}}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle} \right) \]  

(2.22a)

\[ = I - 2 \frac{\vec{B} |\phi\rangle \langle \phi| \vec{B}}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle} + \frac{\vec{B} |\phi\rangle \langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle} \]  

(2.22b)

\[ = I - 2 \frac{\vec{B} |\phi\rangle \langle \phi| B}{\langle \phi| \vec{B} \cdot \vec{B} |\phi\rangle} \]  

(2.22c)

the \( Q \) operator is thus revealed to be a projection operator. Now consider the quantity \( \langle \psi| \vec{A} \cdot \vec{A} |\psi\rangle \)

where \( \vec{A} \) is a Hermitian operator and \( |\psi\rangle \) corresponds to a normalizable state that is not necessarily the same as \( |\phi\rangle \). By its very nature this quantity is non-negative, that is

\[ \langle \psi| \vec{A} \cdot \vec{A} |\psi\rangle \geq 0. \]  

(2.23)

\(^2\)It should be noted that this is a second degree tensor operator.
Now the projection operator $Q$ may be inserted leading to

\[
0 \leq \langle \psi | \hat{A} \cdot Q \cdot Q \cdot \hat{A} | \psi \rangle \tag{2.24a}
\]

\[
= \langle \psi | \hat{A} \cdot Q \cdot \hat{A} | \psi \rangle \tag{2.24b}
\]

\[
= \langle \psi | \hat{A} \cdot \hat{A} | \psi \rangle - \frac{\langle \psi | \hat{A} \cdot \hat{B} | \phi \rangle \langle \phi | \hat{B} \cdot \hat{A} | \psi \rangle}{\langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle} \tag{2.24c}
\]

Multiplying by $\langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle$ yields

\[
\langle \psi | \hat{A} \cdot \hat{A} | \psi \rangle \langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle - \frac{\langle \psi | \hat{A} \cdot \hat{B} | \phi \rangle \langle \phi | \hat{B} \cdot \hat{A} | \psi \rangle}{\langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle} \geq 0 \tag{2.25a}
\]

\[
\langle \psi | \hat{A} \cdot \hat{A} | \psi \rangle \langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle - \langle \psi | \hat{A} \cdot \hat{B} | \phi \rangle \langle \phi | \hat{B} \cdot \hat{A} | \psi \rangle \geq 0 \tag{2.25b}
\]

\[
\langle \psi | \hat{A} \cdot \hat{A} | \psi \rangle \langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle \geq \langle \psi | \hat{A} \cdot \hat{B} | \phi \rangle \langle \phi | \hat{B} \cdot \hat{A} | \psi \rangle. \tag{2.25c}
\]

The result is

\[
\langle \psi | \hat{A} \cdot \hat{A} | \psi \rangle \langle \phi | \hat{B} \cdot \hat{B} | \phi \rangle \geq \left| \langle \psi | \hat{A} \cdot \hat{B} | \phi \rangle \right|^2, \tag{2.26}
\]

which is the Schwarz inequality for dotted operators.

Using the definition for uncertainty of an observable (eq. 2.3) and the square magnitude of the momentum and position (eq. 2.17) allows the expression for the square HTUP to be written as

\[
\left( \Delta \hat{R} \right)^2 \left( \Delta \hat{K} \right)^2 = \frac{\langle \psi | \hat{R} \cdot \hat{R} | \psi \rangle \langle \psi | \hat{K} \cdot \hat{K} | \psi \rangle}{\langle \psi | \psi \rangle^2}. \tag{2.27}
\]

To find the minimum possible value it is necessary to make use of the Schwarz inequality (eq. 2.26), resulting in

\[
\left( \Delta \hat{R} \right)^2 \left( \Delta \hat{K} \right)^2 \geq \left| \frac{\langle \psi | \hat{R} \cdot \hat{K} | \psi \rangle}{\langle \psi | \psi \rangle^2} \right|^2. \tag{2.28}
\]
Now note the product $\mathbf{R} \cdot \mathbf{K}$ may be written as

$$\mathbf{R} \cdot \mathbf{K} = \frac{1}{2} \left( [\mathbf{R} ; \mathbf{K}]_+ + [\mathbf{K} ; \mathbf{R}] \right), \quad (2.29)$$

where $[\mathbf{R} ; \mathbf{K}]_+ = \mathbf{R} \cdot \mathbf{K} + \mathbf{K} \cdot \mathbf{R}$ is the dot product anti-commutator. Making use of the dot product commutator (eq. 2.20) yields

$$\mathbf{R} \cdot \mathbf{K} = \frac{1}{2} \left( [\mathbf{R} ; \mathbf{K}]^2 + 1D^2 \right). \quad (2.30)$$

Substituting this back into equation 2.28 gives

$$\left( \Delta |\mathbf{R}| \right)^2 \left( \Delta |\mathbf{K}| \right)^2 \geq \frac{1}{4} \left( \frac{\langle \psi | [\mathbf{R} ; \mathbf{K}]_+ |\psi \rangle}{\langle \psi | \mathbf{R} \cdot \mathbf{K} |\psi \rangle} \right)^2 + D^2, \quad (2.31)$$

which is the general expression for the HTUP. Equation 2.31 is thus lower bounded by the value $\frac{1}{4}D^2$. The minimum possible value of the HTUP is thus

$$\left( \Delta |\mathbf{R}| \right) \left( \Delta |\mathbf{K}| \right) \geq \frac{1}{2}D. \quad (2.32)$$

### 2.2 Minimum Uncertainty States of the Heisenberg Total Uncertainty Product

It is interesting to examine the conditions that allow the minimum uncertainty to be realized \[4, p286-289\]. One way the conditions can be determined is to find when the dot anti-commutator in equation 2.31 vanishes. When the dot anti-commutator is written out,

$$\langle \psi | [\mathbf{R} ; \mathbf{K}]_+ |\psi \rangle = \langle \psi | \mathbf{R} \cdot \mathbf{K} |\psi \rangle + \langle \psi | \mathbf{K} \cdot \mathbf{R} |\psi \rangle, \quad (2.33)$$
it should be apparent this occurs when

\[ \vec{R} |\psi\rangle = -i\sigma^2 \vec{K} |\psi\rangle \]  
\[ \langle \psi | \vec{R} = i\sigma^2 \langle \psi | \vec{K} , \]  

where \( \sigma^2 \) is an arbitrary real positive number. This is easily verified by

\[ \langle \psi | \vec{R} \cdot \vec{K} |\psi\rangle + \langle \psi | \vec{K} \cdot \vec{R} |\psi\rangle = i\sigma^2 \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle - i\sigma^2 \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle \]
\[ = 0 . \]

When the conditions under which the dot anti-commutator vanishes (eq. 2.34) are used in the Schwarz inequality, the result is

\[ \langle \psi | \vec{R} \cdot \vec{R} |\psi\rangle \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle \geq \langle \psi | \vec{K} \cdot \vec{R} |\psi\rangle \langle \psi | \vec{R} \cdot \vec{K} |\psi\rangle \]  
\[ \sigma^4 \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle = \sigma^4 \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle \langle \psi | \vec{K} \cdot \vec{K} |\psi\rangle , \]

which is the equality condition thus verifying that the minimum value is realized. The really interesting aspect is that equation 2.34 defines a state, \( |\psi\rangle \), under which this is true. Such states belong to a class known as minimum uncertainty states (MUS). The ones under consideration here shall be known as the Minimum Total Uncertainty States (MTUS)

To solve for the minimum uncertainty state, start by expressing equation 2.34 in the momentum representation \( \langle k \rangle \),

\[ \left( i\nabla_{\vec{K}} - \vec{r}_0 \right) \langle k |\psi\rangle = -i\sigma^2 \vec{k} \langle k |\psi\rangle . \]  

(2.37)
Using

\[ \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \vec{1} \nabla_{\vec{K}} \left[ \langle \vec{k} | \psi \rangle \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \right] = \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \left[ \vec{1} \nabla_{\vec{K}} \langle \vec{k} | \psi \rangle \right] \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \] (2.38a)

\[ + \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \langle \vec{k} | \psi \rangle \left[ \vec{1} \nabla_{\vec{K}} \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \right] \] (2.38b)

\[ = \left[ \vec{1} \nabla_{\vec{K}} \langle \vec{k} | \psi \rangle \right] \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \] (2.38c)

\[ - \vec{k} \cdot \langle \vec{k} | \psi \rangle \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \] (2.38d)

allows equation 2.37 to be rewritten as

\[ \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \vec{1} \nabla_{\vec{K}} \left[ \langle \vec{k} | \psi \rangle \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \right] = -\sigma^2 \vec{K} \langle \vec{k} | \psi \rangle \] (2.39a)

\[ \vec{1} \nabla_{\vec{K}} \left[ \langle \vec{k} | \psi \rangle \exp \left( i \vec{r}_0 \cdot \vec{K} \right) \right] = -\sigma^2 \vec{K} \langle \vec{k} | \psi \rangle \exp \left( i \vec{r}_0 \cdot \vec{K} \right) . \] (2.39b)

A solution to this equation is\(^3\)

\[ \langle \vec{k} | \psi \rangle = \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \exp \left( -\frac{\sigma^2}{2} \vec{K}^2 \right) \] (2.40)

in the momentum domain and after taking the Fourier transform

\[ \langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \exp \left( \frac{i}{2\sigma^2} \vec{r} \cdot \vec{r} \right) \exp \left( -\frac{1}{2\sigma^2} \vec{R}^2 \right) \] (2.41)

in the position domain. It can easily be verified,

\[ \left( \Delta \langle \vec{R} \rangle \right)^2 \left( \Delta \langle \vec{K} \rangle \right)^2 = \left( \frac{\sigma^2}{2} D \right) \left( \frac{1}{2\sigma^2} D \right) = \frac{1}{4} D^2 \] (2.42a)

\[ \left( \Delta \langle \vec{R} \rangle \right) \left( \Delta \langle \vec{K} \rangle \right) = \frac{1}{2} D \] (2.42b)

\(^3\) notation note: \( K^2 = \vec{K} \cdot \vec{K} \) and \( R^2 = \vec{R} \cdot \vec{R} \).
that these states are indeed the minimum uncertainty states.

A few of the properties of MTUSs are worth examining here. As can be seen from equations 2.40 and 2.41, the state is Gaussian (multiplied by a phase term) in both the momentum and position representations. The scalar parameter \( \sigma^2 \) controls the width of the Gaussian but is cancelled out in expression for the uncertainty (eq. 2.42). This is just one of the ways that minimum states are not unique. The parameter \( \sigma^2 \) is not a completely arbitrary number. In order for the wavefunction (eq. 2.40 or 2.41) to be normalizable \( \sigma^2 \) must be a positive value (\( \text{Re} \sigma^2 > 0 \)). Attention has so far been restricted to cases of real value \( \sigma^2 \). If this parameter were allowed to be complex, the uncertainty product would be

\[
\frac{D |\sigma^2|}{2 \text{Re} \sigma^2} = \frac{D [\text{Re} \sigma^2 + \text{Im} \sigma^2]}{2 \text{Re} \sigma^2}
\]

which is minimum only when \( \text{Im} \sigma^2 = 0 \). In other words \( \sigma^2 \) is completely real for minimum uncertainty states.

Minimum uncertainty states are also the eigenstates of an annihilation operator [81]. This means there is an operator \( \hat{a} \) with eigenvalue \( \hat{a}_0 \) that results in

\[
(\hat{a} - \hat{a}_0) |\psi\rangle = 0 ,
\]

when \(|\psi\rangle\) is the minimum uncertainty state. The annihilation operator can be identified by starting from the minimization condition (eq. 2.34) rewritten in a slightly different manner as

\[
(\vec{r} - \vec{r}_0) |\psi\rangle = -i \sigma^2 (\vec{k} - \vec{k}_0) |\psi\rangle ,
\]

where \( \vec{r}_0 = \langle \vec{r} \rangle \) and \( \vec{k}_0 = \langle \vec{k} \rangle \). Rearranging the equation gives

\[
(\vec{r} + i \sigma^2 \vec{k}) |\psi\rangle = (\vec{r}_0 + i \sigma^2 \vec{k}_0) |\psi\rangle ,
\]
and dividing by $\sqrt{2}\sigma$ yields
\[ \sqrt{\frac{1}{2}} \left( \frac{\mathbf{r}}{\sigma} + 10\mathbf{k} \right) |\psi\rangle = \sqrt{\frac{1}{2}} \left( \frac{\mathbf{r}_0}{\sigma} + 10\mathbf{k}_0 \right) |\psi\rangle. \] (2.47)

The operator annihilation operator is thus
\[ \overrightarrow{a} = \sqrt{\frac{1}{2}} \left( \frac{\mathbf{r}}{\sigma} + 10\mathbf{k} \right), \] (2.48)

with the complex eigenvalue of
\[ \overrightarrow{a}_0 = \sqrt{\frac{1}{2}} \left( \frac{\mathbf{r}_0}{\sigma} + 10\mathbf{k}_0 \right). \] (2.49)

The adjoint of this annihilation operator is
\[ \overrightarrow{a}^\dagger = \sqrt{\frac{1}{2}} \left( \frac{\mathbf{r}}{\sigma} - 10\mathbf{k} \right), \] (2.50)

which is known as the creation operator. Together these two operators satisfies the usually commutation relation for creation and annihilation pairs [4], as demonstrated by

\[ [\overrightarrow{a}; \overrightarrow{a}^\dagger] = \left( \frac{1}{2} \right) \left[ \left( \frac{\mathbf{r}}{\sigma} + 10\mathbf{k} \right); \left( \frac{\mathbf{r}}{\sigma} - 10\mathbf{k} \right) \right] \] (2.51a)
\[ = \left( \frac{1}{2} \right) \left\{ -1 \left[ \mathbf{r}; \mathbf{k} \right] + i \left[ \mathbf{k}; \mathbf{r} \right] \right\} \] (2.51b)
\[ = \left( \frac{1}{2} \right) \left\{ -i(1D1) + i(-1D1) \right\} \] (2.51c)
\[ = \left( \frac{1}{2} \right) \{D1 + D1\} \] (2.51d)
\[ = D1. \] (2.51e)

It is useful to examine the transformations of the Minimum Total Uncertainty States that leave the uncertainty product (eq. 2.27) unchanged. These transformations are spatial and momentum translations, rotations, inversion, and isotropic dilations of width. Invariance to translations is obvious
when it is realized all the integrals involved,

\[
\frac{\langle \psi | \vec{R} \cdot \vec{R} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{\Sigma_0} d\vec{r} \left( \vec{r} - \vec{r}_0 \right)^2 \exp \left( -\frac{1}{\sigma^2} \left( \vec{r} - \vec{r}_0 \right)^2 \right)}{\int_{\Sigma_0} d\vec{r} \exp \left( -\frac{1}{\sigma^2} \left( \vec{r} - \vec{r}_0 \right)^2 \right)} \tag{2.52a}
\]

\[
\frac{\langle \psi | \vec{K} \cdot \vec{K} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{\Sigma_0} d\vec{k} \left( \vec{k} - \vec{k}_0 \right)^2 \exp \left( -\sigma^2 \left( \vec{k} - \vec{k}_0 \right)^2 \right)}{\int_{\Sigma_0} d\vec{k} \exp \left( -\sigma^2 \left( \vec{k} - \vec{k}_0 \right)^2 \right)}, \tag{2.52b}
\]

are independent of the choice of origin \((\vec{r}_0, \vec{k}_0)\). Likewise, the invariance to rotations and inversion of coordinates are transparent as the integrals transform as scalars under rotation. The individual integrals, however, are not independent of changes to the width parameter, \(\sigma^2\). Physically this invariance is known as squeezing [82] and results in increased resolution of an observable at the expense of its conjugate. For Gaussian states, this can be formulated by introducing a positive real scaling factor \(\lambda\) and replacing \(\sigma^2 \Rightarrow \lambda \sigma^2\). The corresponding annihilation operator,

\[
\left( \vec{R} + \imath \sigma^2 \lambda \vec{K} \right) | \psi \rangle = 0 \tag{2.53}
\]

has the solution of the form

\[
\langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi \sigma^2 \lambda} \right)^{D/2} \exp \left( -\frac{1}{2\sigma^2 \lambda} \vec{R}^2 \right) \tag{2.54a}
\]

\[
\langle \vec{k} | \psi \rangle = \exp \left( -\frac{\sigma^2 \lambda}{2} \vec{K}^2 \right). \tag{2.54b}
\]

The square deviations of position and momentum are thus

\[
\left( \Delta \vec{R} \right)^2 = \left( \frac{\sigma^2 \lambda}{2} D \right) \tag{2.55a}
\]

\[
\left( \Delta \vec{K} \right)^2 = \left( \frac{1}{2\sigma^2 \lambda} D \right), \tag{2.55b}
\]

which shows that \(\lambda < 1\) are squeezed states in \(\vec{R}\), and \(\lambda > 1\) are squeezed states in \(\vec{K}\). Calculating the
uncertainty product,

\[
\left( \Delta \vec{R} \right)^2 \left( \Delta \vec{R} \right)^2 = \left( \frac{\sigma^2 \lambda D}{2} \right) \left( \frac{1}{2\sigma^2 \lambda D} \right) = \frac{1}{4} D^2
\]  

reveals the squeezed states remain minimum uncertainty states. It should be noted that this last type of invariance is distinctive. There are many states that are invariant to translations, rotations, and inversions but relatively few invariant to (isotropic) dilations of the width. This is an important property for squeezed states [83][84] and multi-resolution analysis [85].

In the previous case only isotropic changes to the width parameter, \( \sigma^2 \), were examined. It is instructive to now look at the situation where \( \sigma^2 \) is generalized to the anisotropic case. To illustrate, consider the system of just two degrees of freedom which will be labeled \( x \) and \( y \). Using a different width parameter along each direction results in states of the form:

\[
\Psi(k_x, k_y) = \exp \left( -\frac{1}{2} \left( \sigma^2_x k_x^2 + \sigma^2_y k_y^2 \right) \right)
\]

\[
\psi(x, y) = \left( \frac{1}{2\sigma_x \sigma_y} \right) \exp \left( -\frac{1}{2} \left( \frac{1}{\sigma_x^2} x^2 + \frac{1}{\sigma_y^2} y^2 \right) \right),
\]  

with the corresponding uncertainty product of

\[
U^2 = \frac{1}{\langle \psi | \psi \rangle^2} \langle \psi | (x^2 + y^2) | \psi \rangle \langle \psi | (k_x^2 + k_y^2) | \psi \rangle
\]

\[
= \frac{1}{\langle \psi | \psi \rangle^2} \left( \langle \psi | x^2 | \psi \rangle \langle \psi | k_x^2 | \psi \rangle + \langle \psi | y^2 | \psi \rangle \langle \psi | k_y^2 | \psi \rangle \right)
\]

\[
+ \langle \psi | x^2 | \psi \rangle \langle \psi | k_x^2 | \psi \rangle + \langle \psi | y^2 | \psi \rangle \langle \psi | k_y^2 | \psi \rangle \right) .
\]

To evaluate, look at each type of term separately starting with the \( \langle \psi | x^2 | \psi \rangle / \langle \psi | \psi \rangle \) term. Noting that

\[\]
the degrees of freedom separate\(^5\) permits

\[
\langle \psi | x^2 | \psi \rangle = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx \ x^2 \exp \left( - \left( \frac{1}{\sigma_x^2} x^2 + \frac{1}{\sigma_y^2} y^2 \right) \right) \tag{2.59a}
\]

\[
= \left( \int_{-\infty}^{\infty} dy \exp \left( - \frac{1}{\sigma_y^2} y^2 \right) \right) \left( \int_{-\infty}^{\infty} dx \ x^2 \exp \left( - \frac{1}{\sigma_x^2} x^2 \right) \right) . \tag{2.59b}
\]

With the aid of the definite integral formula

\[
\int_{-\infty}^{\infty} dz \exp (-az^2) = \sqrt{\frac{\pi}{a}} \tag{2.60a}
\]

\[
\int_{-\infty}^{\infty} dz \ z^2 \exp (-az^2) = \frac{\Gamma(3/2)}{a^{3/2}} = \frac{1}{2a^{3/2} \sqrt{\pi}} \tag{2.60b}
\]

where \(\Gamma(\cdots)\) is the gamma function [86], the integrals can be evaluated as

\[
\left( \int_{-\infty}^{\infty} dy \exp \left( - \frac{1}{\sigma_y^2} y^2 \right) \right) = \sigma_y \sqrt{\pi} \tag{2.61}
\]

and

\[
\left( \int_{-\infty}^{\infty} dx \ x^2 \exp \left( - \frac{1}{\sigma_x^2} x^2 \right) \right) = \frac{\sigma_x^3}{2} \sqrt{\pi} . \tag{2.62}
\]

The integral in the denominator

\[
\langle \psi | \psi \rangle = \left( \frac{1}{2\sigma_y \sigma_x \pi} \right) \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx \ \exp \left( - \left( \frac{1}{\sigma_x^2} x^2 + \frac{1}{\sigma_y^2} y^2 \right) \right) \tag{2.63a}
\]

\[
= \left( \frac{1}{2\sigma_y \sigma_x \pi} \right) \left( \int_{-\infty}^{\infty} dy \exp \left( - \frac{1}{\sigma_y^2} y^2 \right) \right) \left( \int_{-\infty}^{\infty} dx \exp \left( - \frac{1}{\sigma_x^2} x^2 \right) \right) \tag{2.63b}
\]

\[
= \left( \frac{1}{2\sigma_y \sigma_x \pi} \right) \sigma_y \sqrt{\pi} \sigma_x \sqrt{\pi} \tag{2.63c}
\]

\[
= 1/2 . \tag{2.63d}
\]

\(^5\) meaning the function \(f(x, y) = g(x)h(y)\), i.e. it may be written as a product of a function of just \(x\) and one of just \(y\).
The \( \langle \psi | x^2 | \psi \rangle / \langle \psi | \psi \rangle \) term is thus

\[
\frac{\langle \psi | x^2 | \psi \rangle}{\langle \psi | \psi \rangle} = 2 \left( \frac{1}{2\sigma_x^2 \sigma_y^2 \pi} \right) \frac{1}{2}\sigma_y^2 \sigma_z^2 \pi \quad \text{(2.64a)}
\]

\[
= \frac{1}{2}\sigma_z^2 . \quad \text{(2.64b)}
\]

Likewise

\[
\frac{\langle \psi | y^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{1}{2}\sigma_y^2 . \quad \text{(2.65)}
\]

Next examine the \( \langle \psi | k_x^2 | \psi \rangle / \langle \psi | \psi \rangle \) term. The numerator of the integral is

\[
\langle \psi | k_x^2 | \psi \rangle = \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_x k_x^2 \exp \left( -\left( \sigma_x^2 k_x^2 + \sigma_y^2 k_y^2 \right) \right) \quad \text{(2.66a)}
\]

\[
= \left( \int_{-\infty}^{\infty} dk_y \exp \left( -\sigma_y^2 k_y^2 \right) \right) \left( \int_{-\infty}^{\infty} dk_x k_x^2 \exp \left( -\sigma_x^2 k_x^2 \right) \right) \quad \text{(2.66b)}
\]

\[
= \left( \frac{1}{\sigma_y \sqrt{\pi}} \right) \left( \frac{1}{2\sigma_x^3 \sqrt{\pi}} \right) \quad \text{(2.66c)}
\]

\[
= \frac{1}{2\sigma_x \sigma_y^2 \pi} \quad \text{(2.66d)}
\]

where the definite integrals 2.61 and 2.62 again have been used. The denominator of the integral is

\[
\langle \psi | \psi \rangle = \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_x \exp \left( -\left( \sigma_x^2 k_x^2 + \sigma_y^2 k_y^2 \right) \right) \quad \text{(2.67a)}
\]

\[
= \frac{1}{\sigma_y \sigma_x \pi} \quad \text{(2.67b)}
\]

making the overall term

\[
\frac{\langle \psi | k_x^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{1}{2} \frac{1}{\sigma_x^2} . \quad \text{(2.68)}
\]

Likewise

\[
\frac{\langle \psi | k_y^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{1}{2} \frac{1}{\sigma_y^2} . \quad \text{(2.69)}
\]
Using these results the uncertainty product simplifies,

\[ U^2 = \frac{1}{\langle \psi | \psi \rangle^2} \left( \langle \psi | x^2 | \psi \rangle \langle \psi | k_x^2 | \psi \rangle + \langle \psi | y^2 | \psi \rangle \langle \psi | k_y^2 | \psi \rangle \right) \]

\[ + \frac{1}{\langle \psi | \psi \rangle^2} \left( \langle \psi | x^2 | \psi \rangle \langle \psi | k_y^2 | \psi \rangle + \langle \psi | y^2 | \psi \rangle \langle \psi | k_x^2 | \psi \rangle \right) \]

\[ = \left( \frac{1}{2} \sigma_x^2 \right) \left( \frac{1}{2} \sigma_2^2 \right) + \left( \frac{1}{2} \sigma_y^2 \right) \left( \frac{1}{2} \sigma_2^2 \right) + \left( \frac{1}{2} \sigma_x^2 \right) \left( \frac{1}{2} \sigma_y^2 \right), \] (2.70a)

with the result

\[ U^2 = \frac{1}{4} \left( 2 + \left( \frac{\sigma_x^2}{\sigma_2^2} + \frac{\sigma_y^2}{\sigma_2^2} \right) \right). \] (2.71)

To better make sense of this result, let \( \sigma_x^2 = c \sigma_y^2 \) where \( c \) is a positive real number. The equation becomes

\[ U^2 = \frac{1}{4} \left( 2 + c + \frac{1}{c} \right). \] (2.72)

Minimizing this expression with respect to \( c \),

\[ \frac{d}{dc} U^2 = \frac{1}{4} \left[ \frac{d}{dc} \right] + \frac{1}{4} \left[ \frac{d}{dc} c^{-1} \right] \]

\[ = 0 = 1 - \frac{1}{c^2} \] (2.73b)

\[ c^2 = 1, \] (2.73c)

reveals the minimum to be \( c = 1 \) or \( \sigma_x^2 = \sigma_y^2 \). The MTUSs are thus characterized by an isotropic width parameter \( \sigma^2 \). Any deviation from the isotopic case results in an increase in uncertainty.

It is worth mentioning that restriction to isotropic width parameters, \( \sigma^2 \), is a distinctive characteristic of MUS of the Heisenberg Total Uncertainty Product. To see this, consider the Robertson uncertainty product for the simple case of two degrees of freedom,

\[ (\Delta x)^2 (\Delta k_x)^2 (\Delta y)^2 (\Delta k_y)^2 \geq \frac{1}{16}. \] (2.74)
It should be apparent that states of the form of equation 2.40 and 2.41 with isotropic $\sigma^2$ minimize this uncertainty product. The difference is that states of the form of equation 2.57 also minimize the Robertson uncertainty product. The MUS derived from the HTUP are thus more restrictive than those derived from the RUP. Although this is a limitation of the MTUS, it is necessary to accept in order to achieve isotropic constrained minimum uncertainty states.

2.3 Constrained Minimum Uncertainty States of the Heisenberg Total Uncertainty Product

Minimum uncertainty states have a number of properties that are desirable in the field of analysis, but they also have a major drawback. For clarity, this discussion will be limited to the specific situation used in later chapters. That is, the approximation of a function and its derivative by a formula of the form

$$\hat{f}(\boldsymbol{r}) = \int_{\mathbb{R}^d} d\boldsymbol{r}' \hat{\phi}(\boldsymbol{r}' - \boldsymbol{r}; M, \sigma) f(\boldsymbol{r}') , \tag{2.75}$$

where $\hat{f}$ is the approximation of the input function $f$, and $\hat{\phi}$ is an approximating identity (or derivative) kernel. The corresponding expression in the momentum domain takes the form

$$\hat{F}(\boldsymbol{k}) = \hat{\Phi}(\boldsymbol{k}) \hat{F}(\boldsymbol{k}) , \tag{2.76}$$

where $F$, $\tilde{F}$, and $\tilde{\Phi}$ are Fourier transforms of $f$, $\tilde{f}$, and $\tilde{\phi}$ respectively. Details of these expressions are discussed in chapter 4, but for now it should be noted they conform to the definition of a filter as discussed in the introduction to this chapter. With this in mind, it will be beneficial to reexamine some filter concepts in more detail. The integral over all space in equation 2.75 is not practical. This can be avoided by using an identity kernel that effectively limits the integration to a small region of space. It should be noted that there is a practical lower limit on the size of this integration volume. The reason for this is the approximation of the derivatives of a function at a point depends on the
value of the neighboring points. The integration volume thus needs to be large enough to include some of the nearby sampled points. When the minimum uncertainty state, which is a Gaussian, is used as the approximating identity kernel the conveniently small localization in position is easily achieved.

Before explaining the drawback of using the MUS it is useful to discuss using the ideal filters as the approximating identity kernel. A comparison of the ideal filter to the Gaussian in the momentum and position domains is depicted in figure 2.2. For the case of an ideal filter, the approximating identity kernel in the momentum domain is unity over a limited range and zero elsewhere. It has the property that, when applied as in equation 2.76, it exactly reproduces the momentum content of the input function that fall under the region where the filter is unity. If almost all the momentum spectra is contained within the window, then the function in the position domain will be well approximated.

The main drawback of the ideal filter is that in the position domain it is a sinc function [87],

\[ \text{sinc}(x) = \frac{\sin(x)}{x} \]

which has infinite variance. The ideal filter is thus impractical to use as an approximating identity kernel. When the effect of the Gaussian filter on the momentum content of a function is considered, its drawback becomes apparent. All momentum, except at the origin, are distorted. A pictorial illustration of this with comparison to the ideal filter can be found in figure 2.2. The resulting approximation to the function may be acceptable but the derivatives, which are more sensitive to momentum content, will be poor.

The shortcomings of using the Gaussian as an approximating identity kernel can be lessened by increasing its width in the momentum domain. This results in more of the momentum spectra being included and a reduction in the amplitude distortion. The natural consequence of this improved representation of the function in the momentum domain is an improvement in position resolution of the function. Even better results would be achieved if the top of the Gaussian could be flattened out to near unity making it more like the ideal filter. It is important that this flattening be done in such a
way as to avoid the infinite spatial variance of the ideal filter. The undesirable spatial delocalization of
the square filter can be traced to the discontinuous change that occurs at its edges. Smoothing out the
edges of a square filter thus results in improved spatial localization. The modifications to the Gaussian
and the ideal filter seem to be describing similar states. One can then easily imagine that a filter that
compromises the two extremes exists (see figure 2.2).

A method that is can produce a compromise between best spatial resolution and phase space local-
ization is constrained minimization of the uncertainty product \[53][54]. The procedure works by first
defining a floor characterized by a known spatial resolution that the minimization process is not allowed
to go below. The minimization itself is analogous to the method of finding the minimum uncertainty
state but this time with respect to a constrained uncertainty product. By proper choice of an initial
state and other restrictions, the resulting constrained minimum uncertainty state (CMUS) will have an
improved resolution in position. Symbolically the improved state is defined by

\[ |\psi_1\rangle = |\psi_0\rangle + |\delta\psi\rangle, \]

where \(|\psi_0\rangle\) is an initial state (or window) and \(|\delta\psi\rangle\) is the change function which will be defined by the
constrained minimization process. By thinking of the improved state as just the \((n-1)^{th}\) function in
the sequence of initial state this procedure can be repeated, as shown by

\[
|\psi_n\rangle = |\psi_{n-1}\rangle + |\delta\psi_n\rangle \quad (2.79a)
= |\psi_0\rangle + \sum_{i=1}^{n} |\delta\psi_n\rangle, \quad (2.79b)
\]

where \(|\delta\psi_n\rangle\) is now a series of step-wise change functions, until a desired degree of spatial resolution is
obtained.

In order to insure that the changes are improvements some restrictions need to be put in place. First
is the normalization convention. Instead of the conventional one of quantum mechanics (the \(L^2\) norm
the one typical for use in filters (the $L^\infty$ norm [89]), that is
\[
\langle \vec{k} | \psi_n \rangle = 1 \text{ at } \vec{k} = \vec{k}_0 ,
\]
will be employed with the normalization in position determined by Fourier transform. A consequence of this is that for the change function
\[
\langle \vec{k} | \delta \psi_n \rangle = 0 \text{ at } \vec{k} = \vec{k}_0 ,
\]
and
\[
\int_{\mathbb{R}^D} d\vec{r}^* e^{-i\vec{k}_0 \cdot \vec{r}^*} \langle \vec{r}^* | \delta \psi_n \rangle = 0 ,
\]
which is the so called admissibility requirement [90]-[92]. Recall that the resolution in position is improved when the state (window) is made wider in the momentum domain; that is, the improved state in momentum domain, $\langle \vec{k} | \psi_n \rangle$, should be wider than the previous state, $\langle \vec{k} | \psi_{n-1} \rangle$. As can been seen from the step-wise procedure in the momentum representation,
\[
\langle \vec{k} | \psi_n \rangle = \langle \vec{k} | \psi_{n-1} \rangle + \langle \vec{k} | \delta \psi_n \rangle ,
\]
this can be guaranteed by using change functions that are everywhere non-negative in momentum space, meaning
\[
\langle \vec{k} | \delta \psi_n \rangle \geq 0 \text{ for all values of } \vec{k} .
\]
To find the quantity subject to the constrained minimization, first consider the square of the uncer-
tainty product for the new state, $|\psi_n\rangle$, which is given by

$$U_n^2 = \left(\Delta \vec{R}\right)_n^2 \left(\Delta \vec{K}\right)_n^2$$

(2.86a)

$$= \frac{1}{\langle \psi_n | \psi_n \rangle^2} \left[ \langle \psi_n | \vec{R} \cdot \vec{R} | \psi_n \rangle \langle \psi_n | \vec{K} \cdot \vec{K} | \psi_n \rangle \right]$$

(2.86b)

where as before $\vec{R} = \vec{r} - \vec{r}_0$ and $\vec{K} = \vec{k} - \vec{k}_0$. Next the floor to the minimization can be defined. Start by expanding the square deviation of momentum in terms of the step-wise change in the uncertainty product,

$$\left(\Delta \vec{K}\right)_n^2 = \frac{1}{\langle \psi_n | \psi_n \rangle} \langle \psi_n | \vec{K} \cdot \vec{K} | \psi_n \rangle$$

(2.87a)

$$= \frac{1}{\langle \psi_n | \psi_n \rangle} \left\{ \langle \psi_{n-1} | \vec{K} \cdot \vec{K} | \psi_{n-1} \rangle + \langle \psi_{n-1} | \vec{K} \cdot \vec{K} | \delta \psi_n \rangle + \langle \delta \psi_n | \vec{K} \cdot \vec{K} | \psi_{n-1} \rangle + \langle \delta \psi_n | \vec{K} \cdot \vec{K} | \delta \psi_n \rangle \right\}$$

(2.87b)

Regrouping into two parts,

$$\left(\Delta \vec{K}\right)_n^2 = \left(\Delta \vec{K}\right)_{nf}^2 + \left(\Delta \vec{K}\right)_{nv}^2$$

(2.88)

where the quantity

$$\left(\Delta \vec{K}\right)_{nv}^2 = \frac{1}{\langle \psi_n | \psi_n \rangle} \langle \delta \psi_n | \vec{K} \cdot \vec{K} | \delta \psi_n \rangle$$

(2.89)

involves just the variation $(\nu)$, $|\delta \psi_n\rangle$, and the quantity

$$\left(\Delta \vec{K}\right)_{nf}^2 = \frac{1}{\langle \psi_n | \psi_n \rangle} \left\{ \langle \psi_{n-1} | \vec{K} \cdot \vec{K} | \psi_{n-1} \rangle \right\}$$

(2.90a)

$$= \frac{1}{\langle \psi_n | \psi_n \rangle} \left\{ \langle \psi_{n-1} | \vec{K} \cdot \vec{K} | \psi_{n-1} \rangle + 2 \text{Re} \left( \langle \psi_{n-1} | \vec{K} \cdot \vec{K} | \delta \psi_n \rangle \right) \right\}$$

(2.90b)

involves the prior state $|\psi_{n-1}\rangle$ as well as the variation. Substituting back into the uncertainty product
It will be required that the quantity \((U^2_n)_f\) be held fixed (f) with respect to the variation, that is

\[
\frac{\delta}{\delta|\delta\psi_n|} (U^2_n)_f = 0 ,
\]

in order to establish the floor to the variation. Since \((U^2_n)_v\), given by

\[
(U^2_n)_v = \frac{1}{(\psi_n|\psi_n)^2} (\psi_n|R-R|\psi_n) (\delta\psi_n|K-K|\delta\psi_n) ,
\]

is inherently non-negative, \((U^2_n)_f\) thus defines a constrained minimum of the uncertainty product,

\[
U^2_n \geq (U^2_n)_f .
\]

Note at this time the actual value of \((U^2_n)_f\) is left undetermined as it contains the variation \(|\delta\psi_n|\). This may seem to be an ill posed problem, but it is analogous to the situation encountered with the Lagrange method of undetermined multipliers\(^6\) [93].

The problem is now to find the variation, \(|\delta\psi_n|\), that minimizes the constrained uncertainty product. This can be achieved by finding the conditions under which \((U^2_n)_v\) (eq. 2.93) takes on its minimal allowed value. This occurs, by making use of the Schwarz inequality

\[
(\psi_n|R-R|\psi_n) (\delta\psi_n|K-K|\delta\psi_n) \geq (\psi_n|R-K|\delta\psi_n) (\delta\psi_n|K-R|\psi_n) ,
\]

\(^6\)In the Lagrange method of undetermined multipliers, the value of the multiplier is not determined until the last step when it is found from the boundary conditions.
when

\[
\begin{align*}
\vec{R} |\psi_n\rangle &= -i\sigma^2 \hat{K} |\delta\psi_n\rangle \\
\langle \psi_n | \vec{R} &= i\sigma^2 \langle \delta\psi_n | \hat{K} ,
\end{align*}
\]  

(2.96a) (2.96b)

where \(\sigma^2\) is an arbitrary real number. To solve for the constrained minimum state, \(|\psi_n\rangle\), and step-wise the change, \(|\delta\psi_n\rangle\), start by looking at the equation in the momentum representation,

\[
\left( i\nabla_{\vec{R}} - \vec{r}_0 \right) \langle \vec{k} | \psi_n \rangle = -i\sigma^2 \hat{K} \langle \vec{k} | \delta\psi_n \rangle .
\]  

(2.97)

The operator on the left hand side can be simplified by introducing a phase factor, to obtain

\[
\begin{align*}
e^{-i\vec{r}_0 \cdot \vec{R}} i\nabla_{\vec{K}} \left[ \langle \vec{k} | \psi_n \rangle e^{i\vec{r}_0 \cdot \vec{K}} \right] \langle \vec{k} | \psi_n \rangle &= -i\sigma^2 \hat{K} \langle \vec{k} | \delta\psi_n \rangle \\
1i\nabla_{\vec{K}} \left[ \langle \vec{k} | \psi_n \rangle e^{i\vec{r}_0 \cdot \vec{K}} \right] &= -i\sigma^2 \hat{K} \langle \vec{k} | \delta\psi_n \rangle e^{i\vec{r}_0 \cdot \vec{K}} .
\end{align*}
\]  

(2.98a) (2.98b)

Making use of substitutions \(\langle \vec{k} | \phi_n \rangle = \langle \vec{k} | \psi_n \rangle e^{i\vec{r}_0 \cdot \vec{K}}\) and \(\langle \vec{k} | \delta\phi_n \rangle = \langle \vec{k} | \delta\psi_n \rangle e^{i\vec{r}_0 \cdot \vec{K}}\) gives

\[
\begin{align*}
i\nabla_{\vec{K}} \langle \vec{k} | \phi_n \rangle &= -i\sigma^2 \hat{K} \langle \vec{k} | \delta\phi_n \rangle \\
\nabla_{\vec{K}} \langle \vec{k} | \phi_n \rangle &= -\sigma^2 \hat{K} \langle \vec{k} | \delta\phi_n \rangle .
\end{align*}
\]  

(2.98c) (2.98d)

Introducing the variable substitution

\[
\xi = \frac{1}{2} \sigma^2 K^2 ,
\]  

(2.99)

converts the problem to the form

\[
\begin{align*}
\left( \nabla_{\vec{K}} : \xi \right) \frac{\partial}{\partial \xi} \langle \vec{k} | \phi_n \rangle &= -\sigma^2 \hat{K} \langle \vec{k} | \delta\phi_n \rangle \\
\sigma^2 \hat{K} \frac{\partial}{\partial \xi} \langle \vec{k} | \phi_n \rangle &= -\sigma^2 \hat{K} \langle \vec{k} | \delta\phi_n \rangle ,
\end{align*}
\]  

(2.100a) (2.100b)
which simplifies to
\[
\frac{\partial}{\partial \xi} \left( \langle k | \varphi_n \rangle \right) = - \langle \overrightarrow{k} | \delta \varphi_n \rangle . \tag{2.101}
\]

At this point an important property of the \textit{improved} state, \( \langle \overrightarrow{k} | \varphi_n \rangle \), can be seen from this equation; that is, when \( \langle \overrightarrow{k} | \delta \varphi_n \rangle \) is everywhere non-negative, as is the case of interest (eq. 2.85), the slope of \( \langle \overrightarrow{k} | \varphi_n \rangle \) must be negative with respect to \( \xi \). In the \( k \) variable this means \( \langle \overrightarrow{k} | \varphi_n \rangle \) is upper bounded by its peak value at \( k = k_0 \) (where \( \langle \overrightarrow{k} | \delta \varphi_n \rangle = 0 \)). As will be seen later, this leads to some desirable consequences. The solution of equation 2.101 can be advanced by using the equation for step-wise change, \( |\varphi_n^{(n)}| = |\varphi_{n-1}^{(n)} + |\delta \varphi_n^{(n)}| \), resulting in
\[
\frac{\partial}{\partial \xi} \langle \xi | \varphi_n \rangle = - \left( \langle \xi | \varphi_n \rangle - \langle \xi | \varphi_{n-1} \rangle \right) \tag{2.102}
\]

which has the solution [2, p442-443]
\[
\varphi_n(\xi) = C e^{-\xi} + \int_0^\xi d\xi' e^{-\xi + \xi'} \varphi_{n-1}(\xi') , \tag{2.103}
\]

where \( C \) is a constant of integration. Recall that the normalization convention (eq. 2.81) sets \( \varphi_n(\xi) = 1 \) at \( \xi = \frac{1}{2} \sigma^2 k_0^2 \) for all \( n \), meaning the constant of integration is \( C = 1 \). The most general form of the CMUS is thus
\[
\varphi_n(\xi) = e^{-\xi} + \int_0^\xi d\xi' e^{-\xi + \xi'} \varphi_{n-1}(\xi') . \tag{2.104}
\]

This equation uniquely specifies the family of step-wise \textit{improved} states, \( \varphi_n(\xi) \), from a chosen initial state \( \varphi_0(\xi) \). With a little manipulation,
\[
\phi_n(\xi) = \varphi_n(\xi) - \varphi_{n-1}(\xi) \tag{2.105a}
\]
\[
= \int_0^\xi d\xi' e^{-\xi + \xi'} \left[ \varphi_{n-1}(\xi') - \varphi_{n-2}(\xi') \right] . \tag{2.105b}
\]
the most general form of the change functions, \( \langle \xi | \delta \varphi_n \rangle \), can be seen to be

\[
\begin{align*}
\phi_1(\xi) &= e^{-\xi} + \int_0^\xi d\xi' e^{-\xi+\xi'} \varphi_0(\xi') - \varphi_0(\xi) & n = 1 \\
\phi_n(\xi) &= \int_0^\xi d\xi' e^{-\xi+\xi'} \phi_{n-1}(\xi') & n \geq 2
\end{align*}
\]  
(2.106)

It is desirable to show that the specifications already in place (eq. 2.81, 2.82, 2.85, 2.101, etc.) are enough to guarantee that the step-wise changes are indeed improvements. Equation 2.85, which specifies that the change function is everywhere non-negative in the momentum representation, assures that the window’s width will increase in momentum. It is instructive to demonstrate that such a change functions exists. Notice from equation 2.106 that if the initial change function, \( \phi_1(\xi) \), is non-negative everywhere then the whole family, \( \phi_n(\xi) \), is also non-negative everywhere. Since the initial change function \( \phi_1(\xi) \) is dependent on the initial state \( \varphi_0(\xi) \), the choice of initial state cannot be arbitrary. It is sufficient that \( \varphi_0(\xi) \) be monotonically decreasing from the origin in order for the initial change function to be non-negative everywhere (see appendix 2B). Recall that the resolution in position is improved when 1) the momentum window is widened and 2) the area over which the window is nearly unity is increased. If the momentum window were made wider but the area over which it was nearly unity was decreased, the resolution in position could actually decrease. For example, an ideal filter could be replaced with a wider Gaussian. It can be demonstrated that this is not possible given the conditions and constraints used here. From equation 2.101 and the discussion that follows it, the improved window \( \langle \xi | \varphi_n \rangle \) is seen to be a monotonically decreasing function with respect to the \( \xi \) coordinate and therefore upper bound by its value at \( \vec{k} = \vec{k}_0 \) in \( \vec{k} \) space. The normalization convention (eq. 2.81) gives the value of this upper bound as 1. Since the change function can only add and only up to the value of 1, the area over which the window is near unity cannot decrease.
It is instructive to look at the example where the square window is the initial state, that is

\[ \varphi_0(\xi) = 1 \quad \text{for } \xi \leq \xi_0, \]
\[ \varphi_0(\xi) = 0 \quad \text{for } \xi > \xi_0, \]

where \( \xi_0 = \frac{1}{2} \sigma^2 a^2 \). Using

\[ \varphi_1(\xi) = e^{-\xi} + \int_0^\xi d\xi' e^{-\xi + \xi'} \varphi_0(\xi'), \]

gives

\[ \varphi_1(\xi) = e^{-\xi} + e^{-\xi} \int_0^\xi d\xi' e^{\xi'} \]  \hspace{1cm} (2.109a)
\[ = e^{-\xi} + (e^{-\xi + \xi} - e^{-\xi}) \]  \hspace{1cm} (2.109b)
\[ = e^{-\xi} (1 - e^{-\xi}) \]  \hspace{1cm} (2.109c)
\[ = 1 \]  \hspace{1cm} (2.109d)

for \( \xi \leq \xi_0 \), and

\[ \varphi_1(\xi) = e^{-\xi} + (e^{-\xi + \xi_0} - e^{-\xi}) \]  \hspace{1cm} (2.110a)
\[ = e^{-\xi + \xi_0} \]  \hspace{1cm} (2.110b)

for \( \xi > \xi_0 \). The results for the first improved state is thus

\[ \varphi_1(\xi) = 1 \quad \text{for } \xi \leq \xi_0, \]
\[ \varphi_1(\xi) = e^{-\xi + \xi_0} \quad \text{for } \xi > \xi_0, \]

(2.111)
and in familiar units (with $T_0 = 0$ and $k_0 = 0$ for simplicity) is

$$\psi_1(k^2) = 1 \quad \text{for} \quad |k| \leq a$$
$$\psi_1(k^2) = \exp \left( -\frac{1}{2} \sigma^2 (k^2 - a^2) \right) \quad \text{for} \quad |k| \geq a$$

(2.112)

where $\xi - \xi_0 = \frac{1}{2} \sigma^2 (k^2 - a^2)$. The result is the square filter with a continuously decaying function appended to its edge (see figure 23.c). Notice that there is also no longer a discontinuity at $|k| = a$, but the first derivative remains discontinuous. Since the area of the window near unity has not been decreased the spatial resolution has not been reduced. The corresponding function in the position domain is shown in figure 2.3.d. It should be noted that this improved function decreases as $|\vec{r}| \to \infty$ at a rate faster than $1/|\vec{r}|$. This process can be repeated with the $n^{th}$ result [54]

$$\varphi_n(\xi) = 1 \quad \text{for} \quad \xi \leq \xi_0$$
$$\varphi_n(\xi) = e^{-\xi + \xi_0} \sum_{j=0}^{n} \frac{(\xi - \xi_0)^j}{j!} \quad \text{for} \quad \xi \geq \xi_0$$

(2.113)

which is a widened state with $n - 1$ continuous derivatives at the point $\xi = \xi_0$. The $n = 13$ improved function in the momentum domain is shown in diagram 2.3.e. Qualitatively it looks like a square window with a half Gaussian appended to its edges. It should also be noticed that the state is wider with the area near unity increased. This is no surprise since

$$\lim_{n \to \infty} \sum_{j=0}^{n-1} \frac{(\xi - \xi_0)^j}{j!} = e^{\xi - \xi_0}$$

(2.114)

meaning

$$\lim_{n \to \infty} \varphi_n(\xi) = e^{-\xi + \xi_0} e^{\xi - \xi_0} = 1$$

(2.115)

that is the improved function converges to unity everywhere. In the position domain (diagram 2.4.f) it should also be noticed the function decreases almost as fast as $e^{-r^2/2\sigma^2}$ giving the state a significant

---

7 The function in the position domain was obtained by computing the inverse Fourier transform numerically on a grid.
degree of spatial localization.

Another choice of initial state that is instructive to look at is generated from the vacuum state,

\[ \varphi_0(\xi) = e^{-\xi}, \quad (2.116) \]

which (recall \( \xi = \frac{1}{2} \sigma^2 K^2 \)) is a Gaussian and hence a minimum uncertainty state. The effect of the first step of the constrained minimization is

\[ \varphi_1(\xi) = e^{-\xi} + e^{-\xi} \int_0^\xi d\xi' \]
\[ = e^{-\xi}(1 + \xi). \quad (2.117) \]

From figure 2.4 it can be seen that qualitatively this state looks like a Gaussian with a flattened top.

The change functions for this choice of initial state are

\[ \phi_1(\xi) = \xi e^{-\xi} \quad (2.118a) \]
\[ \phi_j(\xi) = \frac{\xi^j}{j!} e^{-\xi} \quad (2.118b) \]

and their sum gives the CMUS,

\[ \varphi_n(\xi) = \varphi_0(\xi) + \sum_{j=1}^n \phi_j(\xi) \]
\[ = e^{-\xi} + e^{-\xi} \sum_{j=1}^n \frac{\xi^j}{j!} \]
\[ = e^{-\xi} \sum_{j=0}^n \frac{\xi^j}{j!}. \quad (2.119c) \]

The effect of the step-wise changes is depicted pictorially in figure 2.5. One should notice that

\[ \lim_{n \to \infty} \sum_{j=0}^n \frac{\xi^j}{j!} = e^{+\xi}, \quad (2.120) \]
meaning that
\[
\lim_{n \to \infty} \varphi_n(\xi) = e^{-\xi^2} e^{+\xi} = 1, \tag{2.121}
\]

the CMUS converges to unity everywhere in the momentum domain.

In these examples the starting points were two extremes for states with a given localization in momentum; the square window with best possible resolution in position, and the Gaussian with the best possible simultaneous localization in position and momentum. As can be seen in figure 2.6, that after a number of repeated constrained minimizations both give qualitatively similar results. This suggests a momentum window that is optimal in terms of best resolution and localization in position is square-like in the middle and Gaussian-like at the edges. Of course, in the finite limit the constrained minimum uncertainty state will depend quantitatively on the choice of initial state. For example, it can be seen from equation 2.120 that the CMUS that starts from a Gaussian is equal to unity only at the origin \( \kappa = \kappa_0 \) but can be made arbitrarily close to 1 elsewhere by increasing \( n \). This is in contrast to starting from the square window where the CMUS is exactly equal to unity over a range of momentum values for every \( n \).

2.4 Non-Cartesian Distributed Approximating Functional

Of the two examples of constrained minimum uncertainty states given (eq. 2.113 & 2.119), the one with the Gaussian as the initial state proves to be more practical. The main drawback of the CMUS starting from the square state is for finite \( n \) there are only a finite number of continuous derivatives at the point \( \xi = \xi_0 \). The CMUS starting from a Gaussian is differentiable to all orders, regardless of \( n \). This is obviously a desirable property for numerical applications that rely on derivatives. It should also be recognized that the Gaussian starting point is the minimum uncertainty state (eq. 2.40 & 2.41) of the HTUP. As will be demonstrated, the CMUS starting from the Gaussian retains many of the characteristics of the minimum uncertainty state.

The particular constrained minimum uncertainty state under discussion is known as the Non-
Cartesian Distributed Approximating Functional (NCDAF) \[45\]. Starting from equation 2.119 and working the variable substitutions ($\xi = \frac{1}{2}\sigma^2 k^2$ and $\langle \vec{r} | \psi_n \rangle = \langle \vec{r} | \varphi_n \rangle e^{-i\vec{r} \cdot \vec{K}}$) backwards yields

$$e^{-i\vec{r} \cdot \vec{K}} \hat{\Delta}(\vec{K} - \vec{K}_0; M, \sigma) = e^{-i\vec{r} \cdot \vec{K}} \exp \left(-\frac{\sigma^2}{2} k^2 \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2}{2} k^2 \right)^j ,$$

(2.122)

which is the $M^{th}$ NCDAF in the momentum domain. The corresponding the $M^{th}$ NCDAF in position domain is

$$e^{i\vec{r} \cdot \vec{K}} \hat{\delta}(\vec{r} - \vec{r}_0; M, \sigma, \vec{K}_0) = e^{i\vec{r} \cdot \vec{K}} \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sum_{j=0}^{M} \left( 2\sigma^2 \right)^j \frac{1}{j!} \left( \frac{\sigma^2}{2} k^2 \right)^j \exp \left(-\frac{1}{2\sigma^2} k^2 \right) .$$

(2.123)

The corresponding change functions in the momentum domain are

$$e^{-i\vec{r} \cdot \vec{K}} \phi(\vec{k} - \vec{K}_0; n, \sigma) = e^{-i\vec{r} \cdot \vec{K}} \exp \left(-\frac{\sigma^2}{2} k^2 \right) \frac{1}{n!} \left( \frac{\sigma^2}{2} k^2 \right)^n ,$$

(2.124)

which known as Non-Cartesian Minimum Uncertainty Wavelets (NC 'mu' Wavelets or NC\(\mu\)-Wavelets). The 0\(^{th}\), 1\(^{st}\), and 13\(^{th}\) NCDAFs for the $D = 2$ case are shown in figure 2.7 in both the momentum and position domains. The companion NC\(\mu\)-Wavelets functions are shown in figure 2.8.

An interesting property that has important consequences for numerical application of the NCDAF is that it defines a two-parameter delta functional sequence \[94\]. In the limit where $M \to \infty$

$$\lim_{M \to \infty} \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2}{2} k^2 \right)^j = \exp \left( +\frac{\sigma^2}{2} k^2 \right)$$

(2.125)

and thus

$$\lim_{M \to \infty} \hat{\Delta} = \exp \left( -\frac{\sigma^2}{2} k^2 \right) \exp \left( +\frac{\sigma^2}{2} k^2 \right)$$

(2.126a)

$$= 1$$

(2.126b)
taking the Fourier transform yields
\[
\lim_{M \to \infty} \delta = \delta \left( \vec{r} - \vec{r}_0 \right)
\]  
(2.127)

where \( \delta \) is the delta functional (see figure 2.9). The limit \( \sigma^2 \to 0 \),
\[
\lim_{\sigma^2 \to 0} \exp \left( -\frac{\sigma^2}{2} \frac{K^2}{K^2} \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2}{2} \frac{K^2}{K^2} \right)^j = \lim_{\sigma^2 \to 0} \left( 1 - \frac{\sigma^2}{2} \frac{K^2}{K^2} + \ldots \right) \left( 1 + \frac{\sigma^2}{2} \frac{K^2}{K^2} + \ldots \right)
\]  
(2.128a)
\[
= 1
\]  
(2.128b)

also produces (see figure 2.10)
\[
\lim_{\sigma^2 \to 0} \delta = \delta \left( \vec{r} - \vec{r}_0 \right)
\]  
(2.129)

It is instructive to examine the shape of the NCDAF. For simplicity, just consider cases where \( \vec{r}_0 = 0 \) and \( \vec{k}_0 = 0 \). First, it should be noted that the NCDAF is independent of orientation. The NCDAF in the momentum domain along any axis, for example the x-axis,
\[
\hat{\Delta}(k_x, 0, \ldots, 0; M, \sigma^2) = \exp \left( -\frac{\sigma^2}{2} \frac{(k_x + 0 \ldots + 0)^2}{2} \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2}{2} \frac{(k_x + 0 \ldots + 0)^2}{2} \right)^j ,
\]  
(2.130)
is identical in shape to the one-dimensional DAF,
\[
\hat{\Delta}(k_x; M, \sigma) = \exp \left( -\frac{\sigma^2 k_x^2}{2} \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2 k_x^2}{2} \right)^j .
\]  
(2.131)

The shape in the momentum domain can be characterized by three types of points (see appendix 2C). The first is the inflection points
\[
k_{\text{inflection}} = \frac{\sqrt{2M + 1}}{\sigma},
\]  
(2.132)
along the diameter. The inflection points provide a convenient measure of the width of the momentum window. The second type of points are the maximum curvature points. As can be seen from figure 2.11 these points clearly define the top and base of the momentum plateau. That is, they characterize the
length of the 'Gaussian tail'. Unfortunately, the expression for the location of these points of maximum
curvature is rather complicated (see appendix 2C). A more convenient set of points are the points for
rapid transition,
\[ k_{\text{rapid}}^\pm = \frac{\sqrt{(4M + 3) \pm \sqrt{16M + 9}}}{\sqrt{2\sigma}} \]  
(2.133)
along its diameter, which are also plotted in figure 2.11.

It is useful to examine equations 2.132 and 2.133 scaled by using a width \( \sigma = \sqrt{2M + 1} \). The
equations then become
\[ k_{\text{infection}} = 1 \]  
(2.134)
and
\[ k_{\text{rapid}}^\pm = \frac{\sqrt{(4M + 3) \pm \sqrt{16M + 9}}}{4M + 2} \]  
(2.135)
It can be demonstrated [75] that in the \( M \to \infty \) limit that \( k_{\text{rapid}}^- \to 1 \) and \( k_{\text{rapid}}^+ \to 1 \). This means that
as \( M \) increases the Gaussian tail of the scaled NCDAF momentum window gets steeper. Furthermore,
\( \hat{\Delta}(k_{\text{rapid}}^-) \to 1 \) and \( \hat{\Delta}(k_{\text{rapid}}^+) \to 0 \) as \( M \to \infty \). The scaled NCDAF thus approaches the (isotropic)
ideal window. This is illustrated in figure 2.12.

It is useful to establish some conditions under which one NCDAF momentum window completely
bounds another. Since the shape along the diameter is the same as the one-dimensional case, only
the one-dimensional case needs to be considered. For a fixed value of \( \sigma \), the NCDAF with the greater
\( M \) value will completely bound the other. This is a consequence of the non-crossing rule discussed in
appendix 2B. It states that the curve for a higher \( M \) value can never cross the curve for a lower value
of \( M \). For a fixed value of \( M \), the NCDAF with the smaller value of the width parameter, \( \sigma \), will
completely bound the other. This is a consequence of the NCDAF being a monotonically decreasing
function of distance from origin and the fact that smaller \( \sigma \) means wider momentum windows.

An important property that the NCDAF shares with the minimum uncertainty state is that they
belong to the Schwartz class of functions [95][96]. A Schwartz function is one that decreases in amplitude
to 0 as \(|\mathbf{r}|\to \infty\) faster than any power of \(|\mathbf{r}|\) grows; that is, a Schwartz function multiplied by \(|\mathbf{r}|^n\) for any finite \(n\) vanishes at infinity. Additionally the derivative of a Schwartz function to any order is also a Schwartz function. The concept can be symbolized by

\[
\int_{\mathbb{R}^D} d\mathbf{r} P_n(\mathbf{r}) \left[ \nabla^l_{\mathbf{r}} S(\mathbf{r}) \right] < \infty \quad \text{for any } n, l \in \{0, 1, 2, \ldots\}
\]  

(2.136)

where \(P_n\) is a polynomial in \(\mathbf{r}\) of degree \(n\), \(\nabla^l_{\mathbf{r}}\) is the \(l\)th gradient, and \(S\) is a Schwartz function. The NCDAF can easily be seen to be a member of the Schwartz class from equation 2.123 or 2.122. In the position domain the NCDAF is proportional to the gradient of a Gaussian and in the momentum domain it proportional to a Gaussian multiplied by a finite power series. The consequences of this property will be discussed in section 4.5.5.

It is instructive now to examine the transformations of the NCDAF state that leave their Heisenberg Total Uncertainty Product\(^8\) unchanged. The HTUP for the NCDAF is

\[
(A|A|^2 (A|A|)' = R R \hat{K} \hat{K} \hat{A} \hat{A} \tag{2.137}
\]

where (see appendix 2D) the square variance in position is given by

\[
\left\langle \frac{\Delta |\hat{R}| \hat{R}^\dagger \Delta}{\Delta |\Delta|} \right\rangle = \frac{\sigma^2}{2} \left[ 4 \sum_{j=0}^{M} \frac{1}{2^j} \sum_{j=0}^{M} \frac{1}{2^j} \frac{\Gamma((j+j)+D/2+1)}{\Gamma((j+j)+D/2+1)} \right],
\]

(2.138)

and the square variance in momentum by

\[
\left\langle \frac{\Delta \hat{K} \hat{K} \Delta}{\Delta |\Delta|} \right\rangle = \frac{1}{2\sigma^2} \left[ 4 \sum_{j=0}^{M} \frac{1}{2^j} \sum_{j=0}^{M} \frac{1}{2^j} \frac{\Gamma((j+j)+D/2+1)}{\Gamma((j+j)+D/2+1)} \right].
\]

(2.139)

It is important to note that these square variances are independent of origin and orientation. The\(^8\) The CMUSe are constrained minimum of the HTUP but they are the (absolute) minimum of the constrained uncertainty product (eq. 2.91). This just reflects two different ways of looking at the situation.
NCDAF state is thus invariant to rotations, translations in position and momentum, and inversion of coordinates. It should also be noted that the square variances are dependent on the width parameter $\sigma$; however, the product

$$\frac{\langle \Delta | \mathbf{R} \cdot \mathbf{R} | \Delta \rangle}{\langle \Delta | \Delta \rangle} \frac{\langle \Delta | \mathbf{K} \cdot \mathbf{K} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{\sigma^2}{2} Q_{M,D} \frac{1}{2\sigma^2} P_{M,D}$$

(2.140)

where $Q_{M,D}$ and $P_{M,D}$ are shorthand for the quantities in brackets above (eq. 2.138 & 2.139), is independent of $\sigma$. Like the minimum uncertainty state, the HTUP of the NCDAF states are invariant to isotropic dilations of the width parameter. It should be noted that the HTUP involving the NCDAF states is dependent on anisotropic changes in $\sigma^2$. This is simple to see as the $n = 0$ NCDAF is the minimum uncertainty state of the HTUP and it is not invariant to anisotropic changes in $\sigma^2$.

The uncertainty product of $M^{th}$ NCDAF states is thus invariant to rotations, translations in position and momentum, inversion of coordinates, and isotropic dilations of the width parameter. This is exactly the same set of transformations that characterize the minimum uncertainty states of the Heisenberg Total Uncertainty product. As one might presume the close connection of the NCDAF to Minimum Total Uncertainty States has a lot to do with their Gaussian structure. This Gaussian structure also turns out to be mathematically convenient. The next two chapters make good use of this fact as it is a major advantage for deriving practical expressions for use in numerical applications.
Appendix 2A: Phase and Normalization of Gaussian State in Position Domain

The minimum uncertainty state of the HTUP in the momentum domain has been shown to be

\[
\langle \hat{k} | \psi \rangle = \exp \left( -i \vec{r}_0 \cdot \vec{K} \right) \exp \left( -\frac{\sigma^2}{2} K^2 \right),
\]  

(2A.1)

where \( \vec{K} = \vec{k} - \vec{k}_0 \) and \( \vec{R} = \vec{r} - \vec{r}_0 \). In this appendix it will be demonstrate that the corresponding state in the position domain is

\[
\langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \exp \left( i \vec{k}_0 \cdot \vec{r} \right) \exp \left( -\frac{1}{2\sigma^2} R^2 \right).
\]  

(2A.2)

Since the two are related by a Fourier transform, defined by

\[
F(\vec{k}) = \int_{\mathbb{R}^D} d\vec{r} \exp(-i\vec{k} \cdot \vec{r}) f(\vec{r}),
\]

(2A.3a)

\[
f(\vec{r}) = \left( \frac{1}{2\pi} \right)^D \int_{\mathbb{R}^D} d\vec{k} \exp(-i\vec{k} \cdot \vec{r}) F(\vec{k}),
\]

(2A.3b)

it is the simple matter of performing the inverse Fourier transform on equation 2A.1; symbolically,

\[
\langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi} \right)^D \int_{\mathbb{R}^D} d\vec{k} \exp(+i\vec{k} \cdot \vec{r}) \langle \vec{k} | \psi \rangle
\]

(2A.4a)

\[
= \left( \frac{1}{2\pi} \right)^D \int_{\mathbb{R}^D} d\vec{k} \exp(+i\vec{k} \cdot \vec{r}) \exp(-i\vec{K} \cdot \vec{r}_0) \exp \left( -\frac{\sigma^2}{2} \vec{K}^2 \right).
\]

(2A.4b)

Begin by making the variable change

\[
\begin{align*}
\vec{K} &= \vec{k} - \vec{k}_0 \quad (2A.5a) \\
\vec{dK} &= \vec{dk} \quad (2A.5b)
\end{align*}
\]
to give

\[ \langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi} \right)^D \int_{\mathbb{R}^D} d\vec{K} \exp \left( +1 \left( \vec{k} \cdot \vec{r} - \vec{k}_0 \cdot \vec{r}_0 \right) \right) \exp \left( -\frac{\sigma^2}{2} K^2 \right). \] (2A.6)

The argument of the complex exponential function needs to be evaluated. Using \( \vec{K} = \vec{k} - \vec{k}_0 \) and \( \vec{r} - \vec{r}_0 = \vec{R} \) yields

\[
\begin{align*}
\vec{k} \cdot \vec{r} - \vec{k}_0 \cdot \vec{r}_0 &= \vec{k} \cdot \vec{r} - \vec{k}_0 \cdot \vec{r}_0 - \vec{k}_0 \cdot \vec{r}_0 \\
&= \vec{k} \cdot (\vec{r} - \vec{r}_0) - \vec{k}_0 \cdot \vec{r}_0 \\
&= \vec{k} \cdot \vec{R} - \vec{k}_0 \cdot \vec{r}_0.
\end{align*}
\] (2A.7a)

Inserting this result back into the transform gives

\[ \langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi} \right)^D \exp \left( -1 \vec{k}_0 \cdot \vec{r}_0 \right) \int d\vec{K} \exp \left( +1 \vec{k} \cdot \vec{R} \right) \exp \left( -\frac{\sigma^2}{2} K^2 \right). \] (2A.8)

Furthermore

\[
\begin{align*}
\vec{k} \cdot \vec{R} &= \vec{k} \cdot \vec{R} - \vec{k}_0 \cdot \vec{R} + \vec{k}_0 \cdot \vec{R} \\
&= \left( \vec{k} - \vec{k}_0 \right) \cdot \vec{R} + \vec{k}_0 \cdot \vec{R} \\
&= \vec{k} \cdot \vec{R} + \vec{k}_0 \cdot \vec{R},
\end{align*}
\] (2A.9a)

which lead to

\[ \langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi} \right)^D \exp \left( 1 \left( \vec{k}_0 \cdot \vec{r}_0 + \vec{k}_0 \cdot \vec{R} \right) \right) \int d\vec{K} \exp \left( +i \vec{k} \cdot \vec{R} \right) \exp \left( -\frac{\sigma^2}{2} K^2 \right). \] (2A.10)

Using [97]

\[ \exp \left( -\frac{1}{2\sigma^2} \vec{r}^2 \right) \leftrightarrow FT \Rightarrow (2\pi \sigma^2)^{D/2} \exp \left( -\frac{1}{2} \sigma^2 k^2 \right), \] (2A.11)

allows the integral to be computed, yielding
\[
\langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \exp \left( ik_0 \cdot \left( \vec{r}_0 + \vec{R} \right) \right) \exp \left( -\frac{1}{2\sigma^2} R^2 \right).
\]  

(2A.12)

The phase factor can be simplified by noting that \( \vec{R} + \vec{r}_0 = \vec{r} \), yielding

\[
\langle \vec{r} | \psi \rangle = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \exp \left( ik_0 \cdot \vec{r} \right) \exp \left( -\frac{1}{2\sigma^2} R^2 \right),
\]

(2A.13)

which is the desired result.
Appendix 2B: Possibility of Non-Negative Valued Initial Change Functions

In this appendix it will be demonstrate that if the zeroth DAF, \( \varphi_0(\xi) \), is monotonically decreasing from the origin then the initial change function, \( \phi_1(\xi) \), is non-negative everywhere. First, the non-crossing rule for the zeroth and first DAFs must be established. Postulate that there is a point, \( \xi = \xi_0 \), where \( \varphi_0(\xi) \) and \( \phi_1(\xi) \) are equal. Then the 1st DAF at a point infinitesimally close is of the form

\[
\varphi_1(\xi_0 + \Delta \xi) = \varphi_1(\xi_0) + \Delta \xi \left[ \frac{\partial}{\partial \xi} \varphi_1(\xi) \right]_{\xi=\xi_0},
\] (2B.1)

where \( \Delta \xi \) is an infinitesimal step forward in \( \xi \). From equation 2.102 it is seen

\[
\left[ \frac{\partial}{\partial \xi} \varphi_1(\xi) \right]_{\xi=\xi_0} = -\varphi_1(\xi_0) + \varphi_0(\xi_0)
\] (2B.2)

which from the postulate vanishes. Now

\[
\varphi_1(\xi_0 + \Delta \xi) = \varphi_1(\xi_0),
\] (2B.3)

which at \( \xi = \xi_0 \) is

\[
\varphi_1(\xi_0 + \Delta \xi) = \varphi_1(\xi_0) = \varphi_0(\xi_0).
\] (2B.4)

Given that \( \varphi_0(\xi) \) is a monotonically decreasing function of \( \xi \), then

\[
\varphi_0(\xi_0) > \varphi_0(\xi_0 + \Delta \xi).
\] (2B.5)

This allows one to conclude that

\[
\varphi_1(\xi_0 + \Delta \xi) > \varphi_0(\xi_0 + \Delta \xi).
\] (2B.6)
Thus the first DAF will always be greater than the zeroth DAF except for the point where they touch. Since by the admissibility condition (eq. 2.82) this point occurs at the origin, $\xi_0 = 0$ (and infinity), the two DAFs can never cross. Symbolically the non-crossing rule is

$$\varphi_1(\xi) \geq \varphi_0(\xi) ,$$  \hspace{1cm} (2B.7)

where the equality holds only at the origin and infinity. Now, armed with the non-crossing rule, it is easy to see that 1)

$$-\frac{\partial}{\partial \xi} \varphi_1(\xi) = \varphi_1(\xi) - \varphi_0(\xi) \geq 0 ,$$  \hspace{1cm} (2B.8)

which establishes that the slope of $\varphi_1(\xi)$ must be non-positive everywhere and therefore $\varphi_1(\xi)$ is monotonically decreasing function of $\xi$ and 2)

$$\phi_1(\xi) = \varphi_1(\xi) - \varphi_0(\xi) \geq 0 ,$$  \hspace{1cm} (2B.9)

that is the initial change function is non-negative everywhere.
Appendix 2C: Points of Inflection, Rapid Transition, and Maximum Curvature in the NCDAF Momentum Window

It is the purpose of this appendix identify the location of points of rapid transition and inflection in the NCDAF momentum window. This discussion follows the results of reference [75]. The derivation can greatly be simplified when it is realized that the general NCDAF momentum window along the radius is exactly the same shape as the special case of one degree of freedom. With this in mind attention will be restricted to one degree of freedom.

Begin with the expression for the NCDAF kernel in the momentum domain,

\[ \Delta(k; M, \sigma) = e^{-\sigma^2 k^2/2} \sum_{n=0}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k^2}{2} \right)^n. \]  

(2C.1)

The first derivative of this expression can be determined by direct differentiation,

\[ \frac{d}{dk} \Delta(k; M, \sigma) = \left[ \frac{d}{dk} e^{-\sigma^2 k^2/2} \right] \sum_{n=0}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k^2}{2} \right)^n + e^{-\sigma^2 k^2/2} \sum_{n=0}^{M} \frac{1}{n!} \left[ \frac{d}{dk} \left( \frac{\sigma^2 k^2}{2} \right) \right]^n \]  

(2C.2a)

\[ = -\sigma^2 ke^{-\sigma^2 k^2/2} \sum_{n=0}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k^2}{2} \right)^n + e^{-\sigma^2 k^2/2} \sum_{n=0}^{M} \frac{1}{n!} n \sigma^2 k \left( \frac{\sigma^2 k^2}{2} \right)^{n-1} \]  

(2C.2b)

\[ = -\sigma^2 ke^{-\sigma^2 k^2/2} \left( \sum_{n=0}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k^2}{2} \right)^n - \sum_{n=0}^{M-1} \frac{1}{n!} \left( \frac{\sigma^2 k^2}{2} \right)^n \right) \]  

(2C.2c)

resulting in

\[ \frac{d}{dk} \Delta(k; M, \sigma) = -\sigma^2 k \frac{M}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2/2}. \]  

(2C.3)
Evaluating the second derivative,

\[
\frac{d^2}{dk^2} \tilde{\Delta}(k; M, \sigma) = -\frac{\sigma^2}{M!} \left[ \frac{d}{dk} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \right] - \frac{\sigma^2 k}{M!} \left[ \frac{d}{dk} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \right] \left[ \frac{d}{dk} e^{-\sigma^2 k^2 / 2} \right] = -\frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \left( \frac{\sigma^2 k^2}{2} \right)^{M-1} \frac{d^2}{dk^2} e^{-\sigma^2 k^2 / 2} (2M + 1 - \sigma^2 k^2) \] (2C.4a)

results in

\[
\frac{d^2}{dk^2} \tilde{\Delta}(k; M, \sigma) = -\frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} (2M + 1 - \sigma^2 k^2) , \] (2C.5)

where \( D \) is the number of dimensions. Lastly the expression for the gradient of the Laplacian will be needed. Applying another gradient,

\[
\frac{d^3}{dk^3} \tilde{\Delta}(k; M, \sigma) = -\frac{\sigma^2}{M!} \left[ \frac{d}{dk} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} (2M + 1 - \sigma^2 k^2) \right] - \frac{\sigma^2 k}{M!} \left[ \frac{d}{dk} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \right] \left[ \frac{d}{dk} e^{-\sigma^2 k^2 / 2} \right] \left( \frac{\sigma^2 k^2}{2} \right)^{M-1} \frac{d^2}{dk^2} e^{-\sigma^2 k^2 / 2} (2M + 1 - \sigma^2 k^2) + \frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \left( \frac{\sigma^2 k^2}{2} \right)^{M-2} \frac{d^2}{dk^2} e^{-\sigma^2 k^2 / 2} (2M + 1 - \sigma^2 k^2) \] (2C.6a)

\[
+ \frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M \left[ \frac{d}{dk} e^{-\sigma^2 k^2 / 2} \right] (2M + 1 - \sigma^2 k^2) + \frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M e^{-\sigma^2 k^2 / 2} \left[ \frac{d}{dk} e^{-\sigma^2 k^2 / 2} \right] (2M + 1 - \sigma^2 k^2) \] (2C.6b)

\[
+ \frac{\sigma^2}{M!} \left( \frac{\sigma^2 k^2}{2} \right)^M \left[ \frac{d}{dk} e^{-\sigma^2 k^2 / 2} \right] (2M + 1 - \sigma^2 k^2) + \cdots \] (2C.6c)
\[
\begin{align*}
&= -k \sigma^2 \left( \frac{\sigma^2 k^2}{M!} \right)^M e^{-\sigma^2 k^2/2} \left( \frac{4M^2 + 2M}{k^2} - 2M \sigma^2 \right) \\
&\quad - 2M \sigma^2 - \sigma^2 + \sigma^2 k^2 \sigma^2 - 2\sigma^2 \\
&= -k \sigma^2 \left( \frac{\sigma^2 k^2}{M!} \right)^M e^{-\sigma^2 k^2/2} \left( \frac{4M^2 + 2M}{k^2} - (4M + 1 + 2) \sigma^2 + \sigma^2 k^2 \sigma^2 \right) \quad (2C.6e)
\end{align*}
\]

results in

\[
\frac{d^3}{dk^2} \Delta(k; M, \sigma) = -\sigma^2 k^2 \left( \frac{\sigma^2 k^2}{M!} \right)^M e^{-\sigma^2 k^2/2} \left( \frac{4M^2 + 2M D}{\sigma^2 k^2} - (4M + 1 + 2) \sigma^2 + \sigma^2 k^2 \sigma^2 \right). \quad (2C.7)
\]

The inflection points simply corresponds to the radius in momentum that equation 2C.5 is equal to zero. Simple algebraic manipulation reveals this corresponds to

\[
k^2 = \frac{2M + 1}{\sigma^2}. \quad (2C.8)
\]

The radius corresponding to rapid transitions occurs when equation 2C.7 is equal to zero,

\[
\left( \frac{4M^2 + 2M}{\sigma^2 k^2} - (4M + 3) + \sigma^2 k^2 \right) = 0 \quad (2C.9a)
\]

\[
(4M^2 + 2M) - (4M + 3) \left[ \sigma^2 k^2 \right] + \left[ \sigma^2 k^2 \right]^2 = 0, \quad (2C.9b)
\]

which can be solved for by the quadratic equation,

\[
x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad (2C.10)
\]

with

\[
x = \sigma^2 k^2 \\
a = 1 \\
b = -(4M + 3) \\
c = (4M^2 + 2M) \quad (2C.11)
\]
Working through the algebra, one finds that

\[
\sigma^2 k^2 = \frac{(4M + 3) \pm \sqrt{(4M + 3)^2 - 4(4M^2 + 2M)}}{2},
\]

(2C.12)

which results in radius of rapid transition corresponding to

\[
k^2 = \frac{(4M + 3) \pm \sqrt{16M^2 + 9}}{2}\sigma^2.
\]

(2C.13)

The curvature \[99\] of the momentum window is defined as

\[
\kappa = \left(\frac{d^2}{dk^2} \Delta\right) \left[1 + \left(\frac{d}{dk} \Delta\right)^2\right]^{-3/2},
\]

(2C.14)

where the first and second derivatives are given above (eq. 2C.3 & 2C.5). This expression is maximized where

\[
\frac{d}{dk} \kappa = 0.
\]

(2C.15)

Working through the differentiations yields

\[
0 = \left(\frac{d^2}{dk^2} \Delta\right) \left[1 + \left(\frac{d}{dk} \Delta\right)^2\right]^{-3/2} - 3 \left(\frac{d^2}{dk^2} \Delta\right) \left[1 + \left(\frac{d}{dk} \Delta\right)^2\right]^{-5/2},
\]

(2C.16)

where the third derivative is give by equation 2C.7. The location of the zeros in this equation are best found by employing a numerical root finding technique \[16, p340-386\].
Appendix 2D: Square Variance in Position and Momentum of the NCDAF

In this appendix the square variance in position,

\[ \langle \Delta | R \cdot R | \Delta \rangle / \langle \Delta | \Delta \rangle, \] (2D.1)

and momentum

\[ \langle \Delta | K \cdot K | \Delta \rangle / \langle \Delta | \Delta \rangle, \] (2D.2)

of the NCDAF will be evaluated. It will be convenient to use the momentum representation where the NCDAF is of the form

\[ \langle \vec{k} | \Delta \rangle = \exp \left( -\frac{\sigma^2}{2} K^2 \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \frac{\sigma^2}{2} K^2 \right)^j, \] (2D.3)

where the phase factor has been omitted. It will also be convenient to make the variable substitution of

\[ \vec{\zeta} = \frac{\sigma}{\sqrt{2}} \left( \vec{k} - \langle \vec{K} \rangle \right) = \frac{\sigma}{\sqrt{2}} \vec{K}, \] (2D.4)

which converts the expression to

\[ \langle k | \Delta \rangle = \exp \left( -\vec{\zeta} \cdot \vec{\zeta} \right) \sum_{j=0}^{M} \frac{1}{j!} \left( \vec{\zeta} \cdot \vec{\zeta} \right)^j. \] (2D.5)

This variable change will also effect the integration by

\[ \int_{\mathbb{R}^D} d\vec{k} = \left( \frac{\sqrt{2}}{\sigma} \right)^D \int_{\mathbb{R}^D} d\vec{\zeta}, \] (2D.6)

where \( D \) is the degrees of freedom, and the gradient by

\[ \nabla_{\vec{k}} = \frac{\sigma}{\sqrt{2}} \nabla_{\vec{\zeta}}. \] (2D.7)
The first integral to evaluate is

\[ \langle \Delta | \Delta \rangle = \left( \frac{\sqrt{2}}{\sigma} \right)^D \sum_{i=0}^{M} \frac{1}{i!} \sum_{j=0}^{M} \frac{1}{j!} \int_{\mathbb{R}^D} d\zeta \exp \left( -\zeta^2 \right) \zeta^{2j+2i}. \tag{2D.8} \]

Start by expressing the integration in hyperspherical coordinates \[5\],

\[ \int_{\mathbb{R}^D} d\zeta \exp \left( -\zeta^2 \right) \zeta^{2j+2i} = \int d\Omega \int_0^{\infty} d\zeta \zeta^{D-1} \exp \left( -\zeta^2 \right) \zeta^{2j+2i}, \]

where \( d\Omega \) is the differential element of the set of hyper-angles (\( \Omega \)) and \( \zeta \) is the magnitude of \( \zeta \). Since nothing under the integrand depends on the hyper-angles, they can be integrated over to yield \[98\]

\[ \int d\Omega = \frac{2(\pi)^{D/2}}{\Gamma(D/2)}, \tag{2D.9} \]

where \( \Gamma(\cdots) \) is the gamma function. The integral over the radius is given by

\[ \int_0^{\infty} dx \exp \left( -ax^2 \right) x^m = \frac{\Gamma \left( \frac{m+1}{2} \right)}{2^m \alpha^{(m+1)/2}}, \tag{2D.10} \]

which for this case is

\[ \int_0^{\infty} d\zeta \exp \left( -\zeta^2 \right) \zeta^{2j+2i+D-1} = \frac{1}{2} \frac{\Gamma(i + j + D/2)}{2^{(j+i+D/2)}} \tag{2D.11} \]

Putting the parts back together yields

\[ \langle \Delta | \Delta \rangle = \left( \frac{\sqrt{2}}{\sigma} \right)^D \frac{2(\pi)^{D/2}}{\Gamma(D/2)} \left[ \frac{1}{2} \sum_{j=0}^{M} \frac{1}{j!} \sum_{j=0}^{M} \frac{1}{j!} \frac{\Gamma(i+j+D/2)}{2^{(j+i+D/2)}} \right]. \tag{2D.12} \]

The next integral to evaluate is

\[ \langle \Delta | K K \Delta \rangle = \left( \frac{\sqrt{2}}{\sigma} \right)^D \left( \frac{2}{\sigma^2} \right)^2 \sum_{i=0}^{M} \frac{1}{i!} \sum_{j=0}^{M} \frac{1}{j!} \int_{\mathbb{R}^D} d\zeta \exp \left( -2\zeta^2 \right) \zeta^{2(i+j+1)}. \tag{2D.13} \]
Following similar steps to the last integral reveals it to be

$$\langle \Delta | \mathbf{R} \cdot \mathbf{R} | \Delta \rangle = \left( \frac{\sigma^2}{\sigma} \right)^D \frac{2^{(D/2)}}{\Gamma(D/2)} \left[ \frac{1}{2} \sum_{i=0}^M \frac{1}{i!} \sum_{j=0}^{M} \frac{1}{j!} \Gamma((i+j+D/2+1)) \right]. \quad (2D.14)$$

The last integral to evaluate is

$$\langle \Delta | \mathbf{R} \cdot \mathbf{R} | \Delta \rangle = \left( \frac{\sqrt{2}}{\sigma} \right)^D \frac{\sigma^2\Gamma(D/2)}{2} \int_{\mathbb{R}^D} d\zeta \left\{ \nabla_\zeta \left[ \sum_{i=0}^M \frac{1}{i!} \zeta^{2i} \right] \exp(-\zeta^2) \right\} \cdot \left\{ \nabla_\zeta \left[ \sum_{j=0}^M \frac{1}{j!} \zeta^{2j} \right] \exp(-\zeta^2) \right\}, \quad (2D.15)$$

where \((\cdot)\) denotes the scalar product. The application of the gradient,

$$\nabla_\zeta \left[ \sum_{i=0}^M \frac{1}{i!} \zeta^{2i} \right] \exp(-\zeta^2) = \sum_{i=0}^M \frac{1}{i!} 2i \zeta^{2i-2} - \zeta^2 \left[ \sum_{i=0}^M \frac{1}{i!} \zeta^{2i} \right] \exp(-\zeta^2)$$

$$= -2 \zeta^2 \left[ \sum_{i=0}^M \frac{1}{i!} \zeta^{2i} - \sum_{i=0}^M \frac{1}{(i-1)!} \zeta^{2i-2} \right] \quad (2D.16a)$$

results in

$$\nabla_\zeta \left[ \sum_{i=0}^M \frac{1}{i!} \zeta^{2i} \right] \exp(-\zeta^2) = -2 \zeta^2 \exp(-\zeta^2) \frac{1}{M!} \zeta^{2M}. \quad (2D.17)$$

The integral then becomes

$$\langle \Delta | \mathbf{R} \cdot \mathbf{R} | \Delta \rangle = 4 \left( \frac{\sqrt{2}}{\sigma} \right)^D \frac{\sigma^2\Gamma(D/2)}{2} \frac{1}{M!} \int_{\mathbb{R}^D} d\zeta \exp(-\zeta^2) \zeta^2 \zeta^{4M}. \quad (2D.18)$$

Integration over the hyper-angles and the radius results in

$$\langle \Delta | \mathbf{R} \cdot \mathbf{R} | \Delta \rangle = 4 \left( \frac{\sqrt{2}}{\sigma} \right)^D \frac{\sigma^2\Gamma(D/2)}{2} \frac{1}{M!} \frac{1}{M!} \frac{\Gamma((2M+D/2+1))}{\Gamma((2M+D/2+1))}. \quad (2D.19)$$
The ratio of equations 2D.19 and 2D.12,

\[
\frac{\langle \Delta | \vec{R} \cdot \vec{R} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{4}{2} \left( \frac{s^2}{\sigma} \right) D \frac{2(\pi)^{D/2}}{\Gamma(D/2)} \left[ \frac{1}{2} \sum_{j=0}^{M} \frac{1}{M+1} \right] \frac{\Gamma(2M+D/2+1)}{\Gamma(D/2 + 2M + 1)} \]

(2D.20)

reveals the square variance in position to be

\[
\frac{\langle \Delta | \vec{R} \cdot \vec{R} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{s^2}{2} \left[ \frac{1}{2} \sum_{j=0}^{M} \frac{1}{M+1} \right] \frac{\Gamma(2M+D/2+1)}{\Gamma(D/2 + 2M + 1)} \]

(2D.21)

The ratio of equations 2D.14 and 2D.12,

\[
\frac{\langle \Delta | \vec{K} \cdot \vec{K} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{4}{2} \left( \frac{s^2}{\sigma} \right) D \frac{2(\pi)^{D/2}}{\Gamma(D/2)} \left[ \frac{1}{2} \sum_{j=0}^{M} \frac{1}{M+1} \right] \frac{\Gamma(2M+D/2+1)}{\Gamma(D/2 + 2M + 1)} \]

(2D.22)

yields the square variance in momentum as

\[
\frac{\langle \Delta | \vec{K} \cdot \vec{K} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \left( \frac{\pi}{2\sigma} \right) \left[ \frac{1}{2} \sum_{j=0}^{M} \frac{1}{M+1} \right] \frac{\Gamma(2M+D/2+1)}{\Gamma(D/2 + 2M + 1)} \]

(2D.23)

It is useful to check that these expressions are consistent with the minimum uncertainty state.

Setting \( M = 0 \) and working through the simplifications,

\[
\frac{\langle \Delta | \vec{R} \cdot \vec{R} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{s^2}{2} \left[ \frac{\Gamma(D/2+1)}{\Gamma(D/2)} \right] = \frac{s^2}{2} \left[ \frac{2 \Gamma(D/2 + 1)}{\Gamma(D/2)} \right] = \frac{s^2}{2} \left[ \frac{D \Gamma(D/2)}{2 \Gamma(D/2)} \right] = \frac{s^2}{2} \left( \frac{D}{2} \right) \]

(2D.24a)

(2D.24b)

(2D.24c)

gives the square variance in position of the minimum uncertainty states as

\[
\frac{\langle \Delta | \vec{R} \cdot \vec{R} | \Delta \rangle}{\langle \Delta | \Delta \rangle} = \frac{s^2}{2} D \]

(2D.25)
which is in agreement with equation 2.42. Similarly, the square variance in momentum of the minimum uncertainty state is found to be

\[ \frac{\left\langle \Delta \right| \hat{\mathbf{K}} \cdot \hat{\mathbf{K}} \left| \Delta \right\rangle}{\left\langle \Delta \Delta \right\rangle} = \frac{1}{2\sigma^2} D, \]

(2D.26)

which is also in agreement with equation 2.42.
Figure 2.1: Comparison of the Gaussian (top row), Ideal filter (middle row), and intermediate function (bottom row) in the momentum (left) and position (right) domains.
Figure 2.2: Comparison of the effect of an Ideal filter (b) and a Gaussian (c) on a bandwidth limited function (a).
Figure 2.3: Constrained Minimum Uncertainty State starting from an Ideal filter in momentum and position domains: (a) 0th in momentum, (b) 0th in position, (c) 1st in momentum, (d) 1st in position, (e) 13th in momentum, (f) 13th in position. Dotted lines are enveloping $x^{-1}$ and the dashed lines are Gaussians.
Figure 2.4: Constrained Minimum Uncertainty State starting from a Gaussian in momentum and position domains: (a) $0^{th}$ in momentum, (b) $0^{th}$ in position, (c) $1^{st}$ in momentum, (d) $1^{st}$ in position, (e) $13^{th}$ in momentum, (f) $13^{th}$ in position. Dashed lines are enveloping Gaussians.
Figure 2.5: Constrained Minimum Uncertainty State starting from a Gaussian and the companion change functions: (a) 0th CMUS, (b) 1st Change function, (c) 1st CMUS, (d) 13th change function, and (e) 13th CMUS.
Figure 2.6: Comparison of the 13\textsuperscript{th} Constrained Minimum Uncertainty States starting from an Ideal filter (solid) and a Gaussian (dashed).
Figure 2.7: 0th, 1st, and 13th NCDAF for two degrees of freedom in the momentum ($\Delta$) and position domain ($\delta$).
Figure 2.8: NCDAFs and the companion NCμ-Wavelets: (a) $0^{th}$ NCDAF, (b) $1^{st}$ NCμ-Wavelet, (c) $2^{st}$ NCDAF, (d) $13^{th}$ NCμ-Wavelet, and (e) $13^{th}$ NCDAF.
Figure 2.9: Suggestion of the delta function limit of the NCDAF (kernel) as $M$ is increased. In all cases $\sigma = 1$. 
Figure 2.10: Suggestion of the delta function limit of the NCDAF (kernel) as $\sigma$ is decreased. In all cases $M = 8$. 
Figure 2.11: Location of the points of maximum curvature (+), rapid transition (x), and inflection (*) along the diameter of the NCDAF momentum window. Parameters used were $M = 13$ and $\sigma = 2.0$. 
Figure 2.12: NCDAF momentum window scaled by using $\sigma = \sqrt{2M + 1}$. Values of $M$ used are 1, 2, 4, 8, 16, 32, and 64.
3 The Properties of the Non-Cartesian Distributed Approximating Functional Polynomials and Minimum Uncertainty Wavelets

In chapter 2, the expression for the Non-Cartesian Distributed Approximating Functional (NCDAF) was found to be

\[ \delta(\vec{r} - \vec{r}_0; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sum_{n=0}^{M} \left( \frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \frac{\nabla^2_n}{R} \exp \left( -\frac{1}{2\sigma^2} R^2 \right) \]  

(3.1)

in the position representation, where \( D \) is the number of dimensions, \( \sigma \) is a positive and real valued width parameter, and \( \vec{R} = \vec{r} - \vec{r}_0 \) is the position relative to the origin \( \vec{r}_0 \). It will be shown in this chapter that this equation can be expressed in a convenient polynomial form.

As will be explicitly demonstrated in the next chapter, the derivatives of the NCDAF are directly related to the approximation of the derivatives of a function. For example, the NCDAF approximation of the Laplacian of a function is

\[ \text{NCDAF} \left[ \nabla^2 \right] f(\vec{r}) = \int_{\mathbb{R}^D} d\vec{r}' \delta^{(2)}(\vec{r} - \vec{r}_0; M, \sigma) f(\vec{r}') , \]  

(3.2)

where \( \delta^{(2)} \) is the Laplacian of the NCDAF. Like the NCDAF, the derivatives of the NCDAF can be expressed in a convenient polynomial form. The most important differential operators in the majority of applications (PDE, data analysis, etc.) are the gradient \( \nabla \), the Laplacian \( \nabla^2 \), and combinations thereof. Discussion of derivatives of the NCDAF will thus be limited in this chapter to the gradient and the Laplacian.

The first topic that will be addressed in this chapter is the identification of the NCDAF polynomials. It will be demonstrated that they are closely related to the associated Laguerre polynomials. This fact will be exploited to derive the properties of the NCDAF polynomials that are useful for numerical
applications. Although a number of these properties are not used for the application of the NCDAF approximation formula, they can be used to establish their numerical properties. The next section deals with characterizing the NCμ-Wavelets. As has been shown in chapter 2, the NCDAFs are composed of summations of NCμ-Wavelets. Given this simple inter-relationship, the properties of the NCDAFs can easily be inferred from those of the NCμ-Wavelets. The two important properties that need to be established are the derivative and lowering relationships. As indicated above, the derivative relationships are important to NCDAF derivative approximations. In the final section, the raising and lowering relationships will be viewed in an operator formalism.

3.1 Identification and Characterization of the NCDAF Polynomials

The polynomials that appear in the expression for the NCDAF can most easily be identified from their recursion relationship. Begin by examining the generator expression

$$\left(-\frac{1}{4}\right)^n \frac{1}{n!} \exp\left(+Z^2\right) \nabla^2_n \exp\left(-Z^2\right), \quad (3.3)$$

where $Z = \frac{1}{\sqrt{2f}} (\vec{r} - \vec{r}_0)$ and $\nabla^2_n$ is the $n^{th}$ Laplacian (i.e. $\left(\nabla^2 Z\right)^n$). In order to simplify the derivation, consider first the polynomials generated from just

$$\mathcal{H}_n(Z^2) = \exp\left(+Z^2\right) \nabla^2_n \exp\left(-Z^2\right), \quad (3.4)$$

which are multi-dimensional generalization of the Hermite polynomials\(^\dagger\). It will also be advantageous to work in the Fourier domain (this derivation follows [100], for an alternative methodology see [45]).

\(^\dagger\)see reference [46] (which uses the notation $L_n^\alpha$ for $\mathcal{H}_n^\alpha$)
With this in mind, take the Fourier transform of equation 3.4,

\[ \int_{\mathbb{R}^D} d\mathbf{Z} \ e^{i \mathbf{k} \cdot \mathbf{Z}} H_n(\mathbf{Z}^2) e^{-\mathbf{Z}^2} = \int_{\mathbb{R}^D} d\mathbf{Z} \ e^{i \mathbf{k} \cdot \mathbf{Z}} \nabla_{\mathbf{Z}}^{2n} e^{-\mathbf{Z}^2} \tag{3.5a} \]

\[ = \left( \frac{1}{|k|} \right)^{2n} \int_{\mathbb{R}^D} d\mathbf{Z} \ e^{i \mathbf{k} \cdot \mathbf{Z}} e^{-\mathbf{Z}^2} \tag{3.5b} \]

\[ = (-k^2)^n \int_{\mathbb{R}^C} d\mathbf{Z} \ e^{-\left(\mathbf{Z}^2 - \frac{1}{2} \mathbf{k} \cdot \mathbf{Z} \right)} . \tag{3.5c} \]

To evaluate the right hand side of this equation, it is necessary to complete the square of the exponential function's argument. This is done by

\[ \mathbf{Z}^2 - \mathbf{k} \cdot \mathbf{Z} = \left( \mathbf{Z} - \frac{1}{2} \mathbf{k} \right)^2 + \frac{k^2}{4} \tag{3.6a} \]

\[ = \alpha^2 + \frac{k^2}{4}, \tag{3.6b} \]

where \( \alpha = \mathbf{Z} - \frac{1}{2} \mathbf{k} \). With this result, equation 3.5 becomes

\[ (-k^2)^n \int_{\mathbb{R}^D} d\mathbf{Z} \ e^{-\left(\mathbf{Z}^2 - \frac{1}{2} \mathbf{k} \cdot \mathbf{Z} \right)} = (-k^2)^n e^{-\frac{k^2}{4}} \left( \int_{\mathbb{R}^D} d\alpha \ e^{-\alpha^2} \right) \tag{3.7a} \]

\[ = (-k^2)^n e^{-\frac{k^2}{4}} \left( \pi \right)^{D/2} , \tag{3.7b} \]

and therefore

\[ \int_{\mathbb{R}^D} d\mathbf{Z} \ e^{i \mathbf{k} \cdot \mathbf{Z}} H_{2n}(\mathbf{Z}^2) e^{-\mathbf{Z}^2} = (-1)^n \pi^{D/2} k^{2n} e^{-k^2/4} . \tag{3.8} \]
Next, compute the Laplacian of equation 3.8,

\[ \nabla^2_k \int_{\mathbb{R}^D} d\tilde{Z} \; e^{i\tilde{Z}^T \tilde{J} \tilde{Z}} \mathcal{H}_n^a(\tilde{Z}^2) e^{-\tilde{Z}^2} \]  

(3.9a)

\[ = (-1)^n \pi^{D/2} \nabla^2_k \left[ k^{2n} e^{-k^2/4} \right] \]  

(3.9b)

\[ = (-1)^n \pi^{D/2} \nabla^2_k \left( \left( \nabla^2_k \left[ k^{2n} \right] \right) e^{-k^2/4} + k^{2n} \left[ \nabla^2_k e^{-k^2/4} \right] \right) \]  

(3.9c)

\[ = (-1)^n \pi^{D/2} \nabla^2_k \left( \left( 2n k^{2n-1} \right) e^{-k^2/4} + k^{2n} \left[ \frac{-2}{k} e^{-k^2/4} \right] \right) \]  

(3.9d)

\[ = (-1)^n \pi^{D/2} \left( \nabla^2_k \left[ 2n k^{2n-2} - \frac{1}{2} k^{2n} \right] e^{-k^2/4} \right) \]  

(3.9e)

\[ + \nabla^2_k \left[ 2n k^{2n-2} - \frac{1}{2} k^{2n} \right] e^{-k^2/4} + \nabla^2_k \left[ 2n k^{2n-2} - \frac{1}{2} k^{2n} \right] \left[ \nabla^2_k e^{-k^2/4} \right] \]  

(3.9f)

\[ = (-1)^n \pi^{D/2} \left( D \left[ 2n k^{2n-2} - \frac{1}{2} k^{2n} \right] e^{-k^2/4} + \nabla^2_k \left[ 2n (2n-2) k^{2n-4} - \frac{1}{2} 2n k^{2n-2} \right] e^{-k^2/4} \right) \]  

(3.9g)

\[ + \nabla^2_k \left[ 2n k^{2n-2} - \frac{1}{2} k^{2n} \right] \left[ \frac{-2}{k} e^{-k^2/4} \right] \]  

Collecting the terms with the same power of \( k^2 \) results in

\[ \nabla^2_k \int_{\mathbb{R}^D} d\tilde{Z} \; e^{i\tilde{Z}^T \tilde{J} \tilde{Z}} \mathcal{H}_n^a(\tilde{Z}^2) e^{-\tilde{Z}^2} \]  

(3.10)

\[ = (-1)^n \pi^{D/2} \left( \frac{1}{4} k^{2n+2} - \frac{1}{2} D + 2n \right) k^{2n} + 2n (D + (2n-2)) k^{2n-2} \; e^{-k^2/4} . \]  

Recalling equation 3.8 allows the identification\(^2\) of

\[ \frac{1}{4} (-1)^{n+1} \pi^{D/2} k^{2n+2} e^{-k^2/4} = \frac{1}{4} \int_{\mathbb{R}^D} d\tilde{Z} \; e^{i\tilde{Z}^T \tilde{J} \tilde{Z}} \mathcal{H}_{n+1}^a(\tilde{Z}^2) e^{-\tilde{Z}^2} , \]  

(3.11)

\(^2\)Notice the extra \(-1\) in the first and third expressions.
\[-\left(\frac{1}{2} D + 2n\right) (-1)^n \pi^{D/2} k^{2n} e^{-k^2/4} = -\left(\frac{1}{2} D + 2n\right) \int_{\mathbb{R}^D} d^D z \, e^{i \vec{k} \cdot \vec{z}} \mathcal{H}_{2n}^e (z^2) e^{-z^2}, \quad (3.12)\]

and

\[2n (D + (2n - 2)) (-1)^{n-1} \pi^{D/2} k^{2n} e^{-k^2/4} = 2n (D + 2n - 2) \int_{\mathbb{R}^D} d^D z \, e^{i \vec{k} \cdot \vec{z}} \mathcal{H}_{n-1}^e (z^2) e^{-z^2}. \quad (3.13)\]

All that is needed to determine the recursion is to calculate the inverse transform of the left hand side of equation 3.10, which is

\[\left(\frac{1}{\pi}\right)^{D/2} \int_{\mathbb{R}^D} d \vec{k} \, e^{-i \vec{k} \cdot \vec{z}} \left[ \int_{\mathbb{R}^D} d^D z \, e^{i \vec{k} \cdot \vec{z}} \mathcal{H}_n^e (z^2) e^{-z^2} \right] = -Z^2 \mathcal{H}_n^e (Z^2) e^{-Z^2}. \quad (3.14)\]

Putting the equations together gives

\[-Z^2 \mathcal{H}_n^e (Z^2) e^{-Z^2} = -\frac{1}{4} \mathcal{H}_{n+1}^e (Z^2) e^{-Z^2} - \left(\frac{1}{2} D + 2n\right) \mathcal{H}_n^e (Z^2) e^{-Z^2} - 2n (D + 2n - 2) \mathcal{H}_{n-1}^e (Z^2) e^{-Z^2}. \quad (3.15)\]

With some rearrangement and the common factor $e^{-Z^2}$ removed, the recursion for these polynomials is found to be

\[-\frac{1}{4} \mathcal{H}_{n+1}^e (Z^2) = \left(Z^2 - \frac{1}{2} D - 2n\right) \mathcal{H}_n^e (Z^2) - 2n (D + 2n - 2) \mathcal{H}_{n-1}^e (Z^2). \quad (3.16)\]

Now the remaining factors of the generator expression will be incorporated, by defining

\[L_n(Z^2) = \left(-\frac{1}{4}\right)^n \frac{1}{n!} \mathcal{H}_n^e (Z^2). \quad (3.17)\]
The corresponding recursion relationship becomes

\[ \mathcal{L}_{n+1}(Z^2) = 4 \left( Z^2 - 2n - \frac{D}{2} \right) \mathcal{L}_n(Z^2) \left[ -\frac{1/4}{(n+1)} \right] - 8n \left( D + 2n - 2 \right) \mathcal{L}_{n-1}(Z^2) \left[ \frac{(1/4)^2}{(n+1)n} \right] \]  

(3.18)

\[ (n+1) \mathcal{L}_{n+1}(Z^2) = \left( -Z^2 + 2n + \frac{D}{2} \right) \mathcal{L}_n(Z^2) - \left( \frac{D}{2} + n - 1 \right) \mathcal{L}_{n-1}(Z^2) \]  

(3.19)

A comparison of this expression with the recursion relationship for associated Laguerre polynomials (see appendix 3A),

\[ (n+1) L_{n+1}^{\alpha}(x) = (2n - x + \alpha + 1) L_{n}^{\alpha}(x) - (n + \alpha) L_{n-1}^{\alpha}(x) \]  

(3.20)

reveals that these polynomials are associated Laguerre polynomials with \( \alpha = D/2 - 1 \) and \( x = \bar{z} \cdot \bar{Z} \).

The polynomial generator expression is thus

\[ L_n^{(D/2-1)}(Z^2) = \left( -\frac{1}{4} \right)^n \frac{1}{n!} \exp \left( +Z^2 \right) \nabla^{2n} \exp \left( -Z^2 \right) \]  

(3.21)

and the expression for the NCDAF:

\[ \tilde{\delta}(Z^2; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2) \exp \left( -Z^2 \right) \]  

(3.22)

For convenience a number of useful expressions of the associated Laguerre polynomials are listed in appendix 3A. The reader is referred to [2][101][102] for detailed discussions of their properties. An issue that does need discussion here is the appearance of fractional values in the \( \alpha \) index. In general, fractional indices for associated Laguerre polynomials, present significant difficulties. For example, the expression

\[ L_n^{(\alpha)}(x) = (-1)^\alpha \frac{d^\alpha}{dx^\alpha} L_n^0(x) \]  

(3.23)
faces a major interpretation challenge\textsuperscript{3} for fractional values of $\alpha$. Associated Laguerre functions with non-integer indices are not, in general, polynomials [2, p755]. Fortunately, in the case that appears in the NCDAF expression the difficulties are avoided because the argument $(x)$ is also changed. A problematic equation like the one above (eq. 3.23) becomes

\begin{align*}
L_n^{(\alpha)}(Z^2) &= (-1)^{\alpha} \nabla_{\frac{\partial}{\partial Z}}^\alpha L_{n+\alpha}(Z^2), \\
&= (-1)^{\alpha} \nabla_{\frac{\partial}{\partial Z}}^{2\alpha} \left[ e^{Z^2} \nabla_{\frac{\partial}{\partial Z}}^{2n+2\alpha} Z^{2n+2\alpha} e^{-Z^2} \right],
\end{align*}

(3.24)

(3.25)

where the generator of the ordinary Laguerre polynomials has been used. Half-integer values of $\alpha$ are thus not a difficulty as they appear multiplied by 2 in the derivatives.

There is another useful associated Laguerre polynomial that can be introduced at this time. It is the $L_n^{(D/2)}(Z^2)$ polynomial, which will be seen to be important in the derivative expressions of the NCDAF. It is related to $\alpha = D/2 - 1$ case by the expression (eq. 3A.11)

\begin{equation}
L_n^{(\alpha+1)}(x) = -\frac{d}{dx} L_n^{(\alpha)}(x),
\end{equation}

(3.26)

which with a squared argument becomes

\begin{align*}
\nabla_{\frac{\partial}{\partial Z}} L_n^{(\alpha)}(Z^2) &= \left[ \frac{d}{d[Z^2]} L_n^{(\alpha)}(Z^2) \right] \nabla_{\frac{\partial}{\partial Z}} Z^2 \\
&= 2Z \left[ \frac{d}{d[Z^2]} L_n^{(\alpha)}(Z^2) \right] \\
&= -2Z L_n^{(\alpha+1)}(Z^2).
\end{align*}

(3.27a)

(3.27b)

(3.27c)

For the case under consideration the expression is

\begin{equation}
\frac{\sqrt{Z} L_n^{(D/2)}(Z^2)}{Z} = -\frac{1}{2} \nabla_{\frac{\partial}{\partial Z}} L_n^{(D/2-1)}(Z^2).
\end{equation}

(3.28)

\textsuperscript{3}such an expression however can be given meaning in the realm of fractional Calculus, which is beyond the scope of this discussion.
It should be noted that in equation 3.28 that the $\alpha = D/2$ associated Laguerre appears multiplied by $\overrightarrow{Z}$. As will be seen, this combination is the quantity that is most relevant to the NCDAF. With this in mind, the NCDAF polynomials will be defined as

$$[\overrightarrow{Z}]^i L_n^{(D/2 - 1 + l)}(Z^2),$$

(3.29)

where $[\overrightarrow{Z}]^i$ is the $l^{th}$ rank irreducible Cartesian generated from $\overrightarrow{Z}$ [103]. The two specific types under consideration are

$$
\begin{cases}
L_n^{(D/2 - 1)}(Z^2) & \text{for } l = 0 \\
\overrightarrow{Z} L_n^{(D/2)}(Z^2) & \text{for } l = 1
\end{cases}
$$

(3.30)

Though the mathematical and physical significance of the $l$ index is not important to this discussion, it should be mentioned that the $l$ index is related to the irreducible representation of the hyper-angular momentum group [5]. The relation of the NCDAF polynomials to associated Laguerre is obvious but not trivial. The remainder of this section will be devoted to enumerating the properties of the NCDAF polynomials.
3.1.1 First Few \([\overline{Z}] L_n^{(D/2-1)}(Z^2)\)

The first few polynomials for the \(l = 0\) and \(l = 1\) cases are

\[
\begin{align*}
L_{-1}^{(D/2-1)}(Z^2) &= 0 \\
\overline{Z} L_{-1}^{(D/2)}(Z^2) &= 0 \\
L_0^{(D/2-1)}(Z^2) &= 1 \\
\overline{Z} L_0^{(D/2)}(Z^2) &= \overline{Z} \\
L_1^{(D/2-1)}(Z^2) &= -[Z^2 - \frac{D}{2}] \\
\overline{Z} L_1^{(D/2)}(Z^2) &= -[Z^2 - (\frac{D}{2} + 1)] \overline{Z} \\
L_2^{(D/2-1)}(Z^2) &= \frac{1}{2} [Z^4 - (D + 2)Z^2 + (\frac{1}{4} D^2 + \frac{1}{2} D)] \\
\overline{Z} L_2^{(D/2)}(Z^2) &= \frac{1}{2} [Z^4 - (D + 4)Z^2 + (\frac{1}{4} D^2 + \frac{3}{2} D + 2)] \overline{Z} \\
L_3^{(D/2-1)}(Z^2) &= -\frac{1}{6} [Z^6 - (\frac{3}{2} D + 6)Z^4 + (\frac{3}{4} D^2 + \frac{9}{2} D + 6)Z^2 - (\frac{1}{8} D^3 + \frac{3}{4} D^2 + D)] \\
\overline{Z} L_3^{(D/2)}(Z^2) &= -\frac{1}{6} [Z^6 - (\frac{3}{2} D + 9)Z^4 + (\frac{3}{4} D^2 + \frac{15}{2} D + 18)Z^2 - (\frac{1}{8} D^3 + \frac{3}{4} D^2 + \frac{11}{2} D + 6)] \overline{Z}
\end{align*}
\]

(3.31)

3.1.2 Recursion and Derivative Relationships of \([\overline{Z}] L_n^{(D/2-1)}(Z^2)\)

Most relations are a straight substitution of the relations of those of the associated Laguerre polynomials with \(x = Z^2\) and \(\alpha = D/2 - 1\) or \(D/2\). The recursion for \(\alpha = D/2 - 1\) is simply

\[
(n + 1) L_{n+1}^{(D/2-1)}(Z^2) = (2n - Z^2 + \frac{D}{2}) L_n^{(D/2-1)}(Z^2) - (n + \frac{D}{2} - 1) L_{n-1}^{(D/2-1)}(Z^2) .
\]

(3.32)

Likewise the recursion for the \(\alpha = D/2\) case is

\[
(n + 1) L_{n+1}^{(D/2)}(Z^2) = (2n - Z^2 + \frac{D}{2} + 1) L_n^{(D/2)}(Z^2) - (n + \frac{D}{2}) L_{n-1}^{(D/2)}(Z^2) .
\]

(3.33)
Both of these recursions can be summarized in a general formula

\[(n + 1) L_{n+1}^{(D/2 - 1+i)}(Z^2) = (2n - Z^2 + \frac{D}{2} + l) L_n^{(D/2 - 1+i)}(Z^2) - (n + \frac{D}{2} - 1 + l) L_{n-1}^{(D/2 - 1+i)}(Z^2) \] .

(3.34)

Other recursions include

\[L_n^{(D/2 - 1+i)}(Z^2) = L_n^{(D/2+i)}(Z^2) - L_{n-1}^{(D/2+i)}(Z^2) \] .

(3.35)

\[Z^2 L_n^{(D/2 - 1+i)}(Z^2) = (Z^2 - n) L_n^{(D/2 - 1+i)}(Z^2) - (n + \frac{D}{2} - 1 + l) L_{n-1}^{(D/2 - 1+i)}(Z^2) \] .

(3.36)

\[Z^2 L_{n-1}^{(D/2+i)}(Z^2) = -n L_n^{(D/2 - 1+i)}(Z^2) + (n + \frac{D}{2} - 1 + l) L_{n-1}^{(D/2 - 1+i)}(Z^2) \] .

(3.37)

\[(n + \frac{D}{2} - 1 + l) L_n^{(D/2 - 1+i)}(Z^2) = (n + 1) L_{n+1}^{(D/2 - 1+i)}(Z^2) - (n + 1 - Z^2) L_n^{(D/2 - 1+i)}(Z^2) \] .

(3.38)

Two additional useful recursion relationship not found in standard texts are (see appendix 3B for proof)

\[(n + \frac{D}{2}) L_n^{(D/2 - 1)}(Z^2) = \frac{D}{2} L_n^{(D/2)}(Z^2) - Z^2 L_{n-1}^{(D/2 - 1)}(Z^2) \] .

(3.39)

and (also see appendix 3C for proof)

\[(D - 2Z^2) L_n^{(D/2)}(Z^2) - 2Z^2 L_{n-1}^{(D/2 - 1)}(Z^2) = 2(n + 1) L_{n+1}^{(D/2 - 1)}(Z^2) \] .

(3.40)

Relations involving derivatives are also simple substitutions, provided one realizes that

\[\nabla Z L_n^{(D/2 - 1+i)}(Z^2) = \left[ \frac{d}{d[Z^2]} L_n^{(D/2 - 1+i)}(Z^2) \right] (\nabla Z^2) \] .

(3.41a)

\[= 2Z \left[ \frac{d}{d[Z^2]} L_n^{(D/2 - 1+i)}(Z^2) \right] . \]
The basic derivative relation is thus

\[ \nabla_z L_n^{(D/2-1+l)}(Z^2) = -2Z L_n^{(D/2-1)}(Z^2) \]  

(3.42)

The usefulness of this expression is mainly limited to the \( l = 0 \) case, where it is

\[ \nabla_z L_n^{(D/2-1)}(Z^2) = -2Z L_n^{(D/2)}(Z^2) \]  

(3.43)

as the more relevant derivative for the \( l = 1 \) case is

\[ \nabla_z \left[ Z L_n^{(D/2)}(Z^2) \right] \]  

(3.44)

With this in mind, the cases \( \alpha = D/2 - 1 \) and \( \alpha = D/2 \) will be looked at separately starting with the former. Taking the divergence of equation 3.43 gives

\[ \nabla_z^2 L_n^{(D/2-1)}(Z^2) = -2 \nabla_z \left[ Z L_n^{(D/2)}(Z^2) \right] \]  

(3.45a)

\[ = -2 \left( \left[ \nabla_z \cdot Z \right] L_n^{(D/2)}(Z^2) + Z \cdot \left[ \nabla_z L_n^{(D/2)}(Z^2) \right] \right) \]  

(3.45b)

\[ = -2 \left( DL_n^{(D/2)}(Z^2) - 2Z \cdot Z L_n^{(D/2-1)}(Z^2) \right) \]  

(3.45c)

The right hand side can be simplified by using the recursion relationship 3.39 giving the Laplacian for the \( l = 0 \) case as

\[ \nabla_z^2 L_n^{(D/2-1)}(Z^2) = -4 \left( n - 1 + \frac{D}{2} \right) L_n^{(D/2-1)}(Z^2) \]  

(3.46)
The application of the Laplacian can be repeating $m$ times, resulting in

$$\nabla^2 L_{n}^{(D/2-1)}(Z^2) = \nabla^2 L_{n-2}^{(D/2-1)}(Z^2)$$

$$= -4 \left( n - 1 + \frac{D}{2} \right) \left[ \nabla^2 L_{n-1}^{(D/2-1)}(Z^2) \right]$$

$$= (-4)^2 \left( n - 1 + \frac{D}{2} \right) \left( n - 2 + \frac{D}{2} \right) \left[ \nabla^2 L_{n-2}^{(D/2-1)}(Z^2) \right]$$

$$\vdots$$

$$= (-4)^m \frac{(n - 1 + \frac{D}{2})!}{(n - m - 1 + \frac{D}{2})!} \lambda_{n-m}^{(D/2-1)}(Z^2).$$

Rewritten in terms of gamma functions, the $m^{th}$ Laplacian for the case $l = 0$ is seen to be

$$\nabla^2 L_{n}^{(D/2-1)}(Z^2) = (-4)^m \frac{\Gamma(n + D/2)}{\Gamma(n - m + D/2)} \lambda_{n-m}^{(D/2-1)}(Z^2),$$

where it should be kept in mind that $\lambda_{n-j}^{(D/2-1)} = 0$ for all positive integer values of $j$. Similarly, the $m^{th}$ Laplacian for the $l = 1$ case can be determined. First explicit differentiation of $Z L_{n}^{(D/2)}(Z^2)$ results in

$$\nabla^2 \cdot \left[ Z L_{n}^{(D/2)}(Z^2) \right] = DL_{n}^{(D/2)}(Z^2) - 2Z L_{n}^{(D/2+1)}(Z^2),$$

and using recursion 3.39 gives the gradient for the case $l = 1$ as

$$\nabla^2 \cdot \left[ Z L_{n}^{(D/2)}(Z^2) \right] = 2 \left( n + \frac{D}{2} \right) \lambda_{n-1}^{(D/2-1)}(Z^2).$$

Now the $1^{st}$ Laplacian for the $l = 1$ case will be shown. Taking the divergence of equation 3.50 gives

$$\nabla^2 \left[ Z L_{n}^{(D/2)}(Z^2) \right] = 2 \left( n + \frac{D}{2} \right) \left[ \nabla^2 L_{n}^{(D/2-1)}(Z^2) \right].$$
Using equation 3.43 to evaluate,

$$
\nabla^2_2 \left[ \mathcal{Z} L_{n}^{(D/2)}(Z^2) \right] = 2 \left( n + \frac{D}{2} \right) \left[ -2 \mathcal{Z} L_{n-1}^{(D/2)}(Z^2) \right],
$$

(3.52)

leads to the relation for the Laplacian for the $l = 1$ case as

$$
\nabla^2_2 \left[ \mathcal{Z} L_{n}^{(D/2)}(Z^2) \right] = -4 \left( n + \frac{D}{2} \right) \mathcal{Z} L_{n-1}^{(D/2)}(Z^2).
$$

(3.53)

The $m^{th}$ Laplacian can be determined by repeated applications of the Laplacian,

$$
\nabla^{2m}_2 \left[ \mathcal{Z} L_{n}^{(D/2)}(Z^2) \right] = -4 \left( n + \frac{D}{2} \right) \nabla^{2m-2}_2 \left[ \mathcal{Z} L_{n-1}^{(D/2)}(Z^2) \right]
$$

(3.54a)

$$
= (-4)^2 \left( n + \frac{D}{2} \right) \left( n - 1 + \frac{D}{2} \right) \nabla^{2m-4}_2 \left[ \mathcal{Z} L_{n-2}^{(D/2)}(Z^2) \right]
$$

(3.54b)

$$
\vdots
$$

$$
= (-4)^m \frac{(n + \frac{D}{2})!}{(n - m - 1 + \frac{D}{2})!} \left[ \mathcal{Z} L_{n-m}^{(D/2)}(Z^2) \right].
$$

(3.54c)

When written in terms of gamma functions the expression becomes

$$
\nabla^{2m}_2 \left[ \mathcal{Z} L_{n}^{(D/2)}(Z^2) \right] = (-4)^m \frac{\Gamma(n + D/2 + 1)}{\Gamma(n - m + D/2)} \mathcal{Z} L_{n-m}^{(D/2)}(Z^2),
$$

(3.55)

where it should be kept in mind that $L_{n-m}^{(D/2)} = 0$ for all positive integer values of $m$. Two useful derivative relations remain, that is the gradient of equations 3.48 and 3.55. For the $l = 0$ case, simplifying

$$
\nabla_2 \nabla^{2m}_2 L_{n}^{(D/2-1)}(Z^2) = (-4)^m \frac{\Gamma(n + D/2)}{\Gamma(n - m + D/2)} \left[ \nabla_2 \mathcal{Z} L_{n-m}^{(D/2-1)}(Z^2) \right]
$$

(3.56a)

with the aid of equation 3.43 gives

$$
= (-4)^m \frac{\Gamma(n + D/2)}{\Gamma(n - m + D/2)} \left[ -2 \mathcal{Z} L_{n-m-1}^{(D/2)}(Z^2) \right].
$$

(3.56b)
The result shows the gradient of the $m^{th}$ Laplacian for the $l = 0$ case to be

$$
\nabla_Z \nabla^2_Z L_n^{(D/2-1)}(Z^2) = -2 (-4)^m \frac{\Gamma(n + D/2 + 1)}{\Gamma(n - m + D/2)} \nabla_Z L_{n-m}^{(D/2)}(Z^2). \tag{3.57}
$$

Similarly, for the $l = 1$ case, simplifying

$$
\nabla_Z \nabla^2_Z \left[ Z L_n^{(D/2)}(Z^2) \right] = (-4)^m \frac{\Gamma(n + D/2 + 1)}{\Gamma(n - m + D/2)} \nabla_Z \left[ Z L_{n-m}^{(D/2)}(Z^2) \right] \tag{3.58a}
$$

by using equation 3.50 gives

$$
= (-4)^m \frac{\Gamma(n + D/2 + 1)}{\Gamma(n - m + D/2)} \left[ 2 \left(n - m + \frac{D}{2}\right) L_{n-m}^{(D/2-1)}(Z^2) \right]. \tag{3.58b}
$$

So the gradient of the $m^{th}$ Laplacian for the $l = 1$ case is

$$
\nabla_Z \nabla^2_Z \left[ Z L_n^{(D/2)}(Z^2) \right] = 2 \left(n - m + \frac{D}{2}\right) (-4)^m \frac{\Gamma(n + D/2 + 1)}{\Gamma(n - m + D/2)} L_{n-m}^{(D/2-1)}(Z^2). \tag{3.59}
$$

### 3.1.3 Values of $L_n^{(D/2-1)}(Z^2)$ at $Z^2 = 0$

In order to demonstrate the completeness of the NCDAF approximation in the next chapter it will be useful to know the value of $L_n^{(D/2-1)}$ at the zero of its argument$^4$, that is, when $Z^2 = 0$. Inserting the value $\alpha = D/2 - 1$ into the general equation 3A.12 gives

$$
L_n^{(D/2-1)}(0) = \frac{1}{n!} \left(n - 1 + \frac{D}{2}\right)!, \tag{3.60}
$$

which in terms of gamma functions is

$$
L_n^{(D/2-1)}(0) = \frac{\Gamma(n + D/2)}{n! \Gamma(D/2)}. \tag{3.61}
$$

$^4$ $Z L_n^{(D/2)}(Z^2)$ evaluated at $Z^2 = 0$ are all obviously equal to 0.
3.1.4 Orthogonality of $[\vec{Z}] L_n^{(D/2-1+1)}(Z^2)$

For associated Laguerre polynomials with $\alpha = D/2 - 1 + 1$ and $\chi = Z^2$ the orthogonality expression takes the form

$$\int_{R^D} d\vec{Z} Z^{2l} L_n^{(D/2-1+1)}(Z^2) L_n^{(D/2-1+1)}(Z^2) \exp(-Z^2).$$

(3.62)

Since the integrand depends only on the magnitude of the vector $\vec{Z}$, it is advantageous to separate out the hyper-angles from the integration. This is done by noting that

$$\int_{R^D} d\vec{Z} = \int d\Omega \int_0^\infty dZ Z^{D-1},$$

(3.63)

where $d\Omega$ is the differential element of the set of hyper-angles ($\Omega$) and $Z$ is the magnitude of $\vec{Z}$. Using

$$\int d\Omega = \frac{2}{\Gamma(D/2)} (\pi)^{D/2},$$

(3.64)

allows the expression to be rewritten as

$$\frac{2}{\Gamma(D/2)} (\pi)^{D/2} \int_0^\infty dZ Z^{2l+D-1} L_n^{(D/2-1+1)}(Z^2) L_n^{(D/2-1+1)}(Z^2) \exp(-Z^2).$$

(3.65)

Now making the variable substitution

$$\chi = Z^2$$

(3.66a)

$$d\chi = 2ZdZ,$$}

(3.66b)

results in

$$\frac{2}{\Gamma(D/2)} (\pi)^{D/2} \frac{1}{2} \int_0^\infty d\chi \chi^{D/2-1+1} L_n^{(D/2-1+1)}(\chi) L_n^{(D/2-1+1)}(\chi) \exp(-\chi).$$

(3.67)
The integral can now be computed with the standard associated Laguerre orthogonality expression (eq. 3A.13) yielding

$$
\int_{R^D} d\vec{z} Z^{2i} L^{(D/2-1+i)}_n(Z^2) L^{(D/2-1+i)}_m(Z^2) \exp(-Z^2) = \frac{1}{n!} \frac{\Gamma(n+D/2)}{\Gamma(D/2)} \pi^{D/2} \delta_{n,m}
$$

or specifically for the $l = 0$ case

$$
\int_{R^D} d\vec{z} L^{(D/2-1)}_n(Z^2) L^{(D/2-1)}_m(Z^2) \exp(-Z^2) = \frac{1}{n!} \frac{\Gamma(n+D/2)}{\Gamma(D/2)} \pi^{D/2} \delta_{n,m}
$$

(3.68)

and for the $l = 1$ case

$$
\int_{R^D} d\vec{z} L^{(D/2)}_n(Z^2) L^{(D/2)}_m(Z^2) Z^2 \exp(-Z^2) = \frac{1}{n!} \frac{\Gamma(n+1+D/2)}{\Gamma(D/2)} \pi^{D/2} \delta_{n,m}
$$

(3.69)

Lastly, it is apparent that the overlap integral of $\alpha = D/2 - 1$ and $D/2$ for any choice of $n$ and $m$ is

$$
\int_{R^D} d\vec{z} L^{(D/2-1)}_n(Z^2) (L^{(D/2)}_m(Z^2) \vec{z}) \exp(-Z^2) = 0
$$

(3.70)

### 3.1.5 Completeness of $L^{(D/2-1+i)}_m(Z^2)$

The set of associated Laguerre polynomials

$$
\left\{ L^{(\alpha)}_n(x) \mid n = 0, 1, \cdots \infty \right\},
$$

(3.71)

is complete for any function of $x$ in the region $x = [0, \infty)$. This means that the set

$$
\left\{ L^{(D/2-1)}_n(Z^2) \mid n = 0, 1, \cdots \infty \right\},
$$

(3.72)
is complete for any function of , that is, a function that transforms as a scalar upon rotation of the coordinates. By similar reasoning, the set

\[ \left\{ \vec{\mathcal{L}} L_n^{(D/2)}(Z^2) \mid n = 0, 1, \cdots \infty \right\}, \quad (3.73) \]

is complete for any function that transforms as a vector upon rotation of the coordinates.

3.2 Characterization of the NCμ-Wavelets

We now turn our attention to examining the important properties of the NCμ-Wavelets. Using the expressions for the NCDAF polynomials, the expression for the NCμ-Wavelet can be written as

\[ \phi_n^{(D/2-1+i)}(\vec{Z}) = [\vec{\mathcal{L}}] L_n^{(D/2-1+i)}(Z^2) e^{-Z^2}, \quad (3.74) \]

where and \( I = 0, 1 \) for the 0th and 1st NCμ-Wavelets respectively. Of all the properties, the most important for numerical applications are the derivative relationships. Key to the derivations of these derivative relationships are the generator expressions of the NCμ-Wavelets and hence they will be discussed first. After the derivative relationships are detailed, the lowering relationships will be derived. As will be seen in the next section, the lowering and derivative relationships cast in an operator formalism will lead to physical insight of the NCμ-Wavelets.

3.2.1 Generator Expressions for \( [\vec{\mathcal{L}}] L_n^{(D/2-1+i)}(Z^2) e^{-Z^2} \)

The generator expression for \( n^{th} \) polynomial for the \( l = 0 \) case is

\[ L_n^{(D/2-1)}(Z^2) \exp(-Z^2) = (-\frac{1}{4})^n \frac{1}{n!} \nabla^{2n}_Z \exp(-Z^2), \quad (3.75) \]
which is a trivial rearrangement of the polynomial generator expression (eq. 3.21). The $l = 1$ case can be easily found by taking the gradient of equation 3.75,

$$
\nabla Z \left[ L_n^{(D/2-1)}(Z^2) \exp(-Z^2) \right] = \left[ \nabla Z L_n^{(D/2-1)}(Z^2) \right] \exp(-Z^2) + L_n^{(D/2-1)}(Z^2) \left[ \nabla Z \exp(-Z^2) \right]
$$

(3.76a)

$$
= -2Z L_n^{(D/2)}(Z^2) \exp(-Z^2) - 2Z L_n^{(D/2-1)}(Z^2) \exp(-Z^2)
$$

(3.76b)

$$
= -2Z \left\{ L_n^{(D/2)}(Z^2) + L_n^{(D/2-1)}(Z^2) \right\} \exp(-Z^2).
$$

(3.76c)

The quantity in \{\ldots\} brackets is given by equation 3.35, so the expression for the generator of the $n^{th}$ polynomial for the $l = 1$ case is thus

$$
\nabla Z L_n^{(D/2)}(Z^2) \exp(-Z^2) = -\frac{1}{2} \left( \frac{-1}{4} \right)^n \frac{1}{n!} \nabla Z \nabla^{2n} \exp(-Z^2).
$$

(3.77)

Alternatively, this expression may be rearranged by using

$$
\nabla Z L_n^{(D/2)}(Z^2) \exp(-Z^2) = \frac{1}{2} \left( \frac{-1}{4} \right)^n \frac{1}{n!} \nabla Z \nabla^{2n} \left\{ \nabla Z \exp(-Z^2) \right\},
$$

(3.78)

to give a different version of the generator of the $n^{th}$ polynomial for the $l = 1$ case as

$$
\nabla Z L_n^{(D/2)}(Z^2) \exp(-Z^2) = -\left( \frac{-1}{4} \right)^n \frac{1}{n!} \nabla Z \nabla^{2n} \left\{ \nabla Z \exp(-Z^2) \right\}.
$$

(3.79)
3.2.2 Derivative Relations of $\left[ \frac{Z}{Z} \right] L_n^{(D/2-1)}(Z^2)e^{-Z^2}$

With the aid of the generator expressions, the gradients of the NC$\mu$-Wavelets can be established. Begin by rearranging the generator for the $l = 0$ case (eq. 3.75) as

$$L_n^{(D/2-1)}(Z^2)e^{-Z^2} = -2 \left( -\frac{1}{4} \right) \frac{(n-1)!}{n!} \nabla Z \cdot \left\{ -\frac{1}{2} \left( -\frac{1}{4} \right)^{n-1} \frac{1}{(n-1)!} \nabla Z \nabla^2 Z e^{-Z^2} \right\} . \quad (3.80)$$

It should be recognized (by using eq. 3.77) that the function inside the \{\cdots\} brackets is

$$\frac{-1}{2} \left( -\frac{1}{4} \right)^{n-1} \frac{1}{(n-1)!} \nabla Z \nabla^2 Z e^{-Z^2} = \nabla Z L_n^{(D/2)}(Z^2)e^{-Z^2} , \quad (3.81)$$

making the overall expression

$$L_n^{(D/2-1)}(Z^2)e^{-Z^2} = \frac{1}{2n} \nabla Z \left\{ \nabla Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} . \quad (3.82)$$

Shifting the $n$ index of this equation up by 1 results in the gradient for $l = 1$ NC$\mu$-Wavelet,

$$\nabla Z \left\{ \nabla Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = 2 (n + 1) L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2} . \quad (3.83)$$

Likewise, rearranging the generator equation 3.77 and comparing with equation 3.75 yields

$$\nabla Z L_n^{(D/2)}(Z^2)e^{-Z^2} = -\frac{1}{2} \nabla Z \left\{ \left( -\frac{1}{4} \right)^n \frac{1}{n!} \nabla^2 Z e^{-Z^2} \right\} \quad (3.84a)$$

$$= -\frac{1}{2} \nabla Z \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} . \quad (3.84b)$$

The gradient for the $l = 0$ case is thus

$$\nabla Z \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = -2 \nabla Z L_n^{(D/2)}(Z^2)e^{-Z^2} . \quad (3.85)$$
It should be noted, for future reference, that the gradient of the $l=0$ NC$\mu$-Wavelet is proportional to the $l=1$ NC$\mu$-Wavelet, and visa versa.

The Laplacian can similarly be found. Starting from a rearranged version of generator expression 3.75,

\begin{equation}
L^{(D/2-1)}_n(Z^2)e^{-Z^2} = \left(-\frac{1}{4}\right) \frac{(n-1)!}{n!} \nabla_Z^2 \left\{ \left(-\frac{1}{4}\right)^{n-1} \frac{1}{(n-1)!} \nabla^{2n-2}_Z e^{-Z^2} \right\} \tag{3.86a}
\end{equation}

\begin{equation}
= \left(-\frac{1}{4}\right) \frac{1}{n} \nabla_Z^2 \left\{ L^{(D/2-1)}_{n-1}(Z^2)e^{-Z^2} \right\}. \tag{3.86b}
\end{equation}

When the $n$ index is shifted up by one, the Laplacian of the $l=0$ NC$\mu$-Wavelet is found to be

\begin{equation}
\nabla_Z^2 \left\{ L^{(D/2-1)}_n(Z^2)e^{-Z^2} \right\} = -4(n+1) L^{(D/2-1)}_{n+1}(Z^2)e^{-Z^2}. \tag{3.87}
\end{equation}

It should be noted that the Laplacian of the $(n^{th}, l=0)$ NC$\mu$-Wavelet is proportional to the $((n+1)^{th}, l=0)$ NC$\mu$-Wavelet. Following the same procedure for the $l=1$ case,

\begin{equation}
\nabla_Z L^{(D/2)}_n(Z^2)e^{-Z^2} = \left(-\frac{1}{4}\right) \frac{(n-1)!}{n!} \nabla_Z^2 \left\{ \frac{1}{2} \left(-\frac{1}{4}\right)^{n-1} \frac{1}{(n-1)!} \nabla^{2n-1}_Z e^{-Z^2} \right\} \tag{3.88a}
\end{equation}

\begin{equation}
= \left(-\frac{1}{4}\right) \frac{1}{n} \nabla_Z^2 \left\{ \nabla_Z L^{(D/2)}_{n-1}(Z^2)e^{-Z^2} \right\}, \tag{3.88b}
\end{equation}

yields the Laplacian of the $l=1$ NC$\mu$-Wavelet as

\begin{equation}
\nabla_Z^2 \left\{ \nabla_Z L^{(D/2)}_n(Z^2)e^{-Z^2} \right\} = -4(n+1) \nabla_Z L^{(D/2)}_{n+1}(Z^2)e^{-Z^2}. \tag{3.89}
\end{equation}

Analogous to the $l=0$ case, the Laplacian of the $(n^{th}, l=1)$ NC$\mu$-Wavelet is proportional to the $((n+1)^{th}, l=1)$ NC$\mu$-Wavelet. Thus, a closed inter-relationship between the $l=0$ and 1 NC$\mu$-Wavelets has been demonstrated. That is, the gradient of one produces the other, and the Laplacian returns the same NC$\mu$-Wavelet with a shifted index.
This process can be repeated to determine higher orders of Laplacians. First consider just the \( l = 0 \) case. Taking advantage of the previous results, rewrite the expression for the \( m^{th} \) Laplacian in the following manner,

\[
\nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = \nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\}.
\]

The Laplacian of the quantity in the brackets is given by equation 3.87, so the above equation simplifies to

\[
\nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = -4(n+1) \nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\}.
\]

Repeating this procedure,

\[
-4(n+1) \nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\}
\]

allows the general expression for the \( m^{th} \) Laplacian of the \( l = 0 \) NC\( \mu \)-Wavelet to be deduced as

\[
\nabla^2 \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = (-4)^m \frac{(n+m)!}{n!} L_n^{(D/2-1)}(Z^2)e^{-Z^2}.
\]

The effect of the \( m \) Laplacians on the \( (n,l = 0) \) NC\( \mu \)-Wavelet is thus the \( (n+m)^{th}, l = 0 \) NC\( \mu \)-Wavelet with a multiplicative factor that depends on \( n \) and \( m \). Now consider the \( l = 1 \) case. Following
the same procedure,

\[ \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = -4(n + 1) \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_{n+1}^{(D/2)}(Z^2)e^{-Z^2} \right\} = -4(n + 1) \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_{n+1}^{(D/2)}(Z^2)e^{-Z^2} \right\} = (-4)^2(n + 1)(n + 2) \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} \frac{Z}{Z} L_{n+2}^{(D/2)}(Z^2)e^{-Z^2} \right\} \]

allows one to deduce the general expression for the \(m\)th Laplacian of the \(l = 1\) NC\(\mu\)-Wavelet as

\[ \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = (-4)^m \frac{(n+m)!}{n!} \frac{Z}{Z} L_{n+m}^{(D/2)}(Z^2)e^{-Z^2} \].

The \(m\)th Laplacian of the \((n^th, l = 1)\) NC\(\mu\)-Wavelet is thus the \(((n + m)^th, l = 1)\) NC\(\mu\)-Wavelet with a multiplicative factor that depends on just \(n\) and \(m\).

Lastly, the gradients of the \(m\)th Laplacians can be determined. Since the Laplacian and the gradient commute, one can switch their order giving the \(m\)th Laplacian of the gradient as

\[ \nabla^2 \frac{Z}{Z} \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = \nabla^2 \frac{Z}{Z} \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} \quad \text{for } l = 0 \]
\[ \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} \quad \text{for } l = 1 \]

The gradients of the quantities in the brackets are given by equation 3.85 and 3.83, producing

\[ \nabla^2 \frac{Z}{Z} \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = -2 \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} \quad \text{for } l = 0 \]
\[ \nabla^2 \frac{Z}{Z} \left\{ \frac{Z}{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = 2(n + 1) \nabla^2 \frac{Z}{Z} \left\{ L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2} \right\} \quad \text{for } l = 1 \]
Using equations 3.48 and 3.95, yields the gradients of the \(m\)th Laplacians for the \(l = 0\) NC\(\mu\)-Wavelet as

\[
\nabla \frac{\partial}{\partial Z} \frac{\partial^{2m}}{\partial Z^2} \left\{ L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\} = -2 (-4)^{m} \frac{(n+m)!}{n!} L_{n+m}^{(D/2)}(Z^2)e^{-Z^2} ,
\]

and the expressions for the \(l = 1\) NC\(\mu\)-Wavelet as

\[
\nabla \frac{\partial}{\partial Z} \frac{\partial^{2m}}{\partial Z^2} \left\{ \frac{Z}{2} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = 2 (-4)^{m} \frac{(n+m+1)!}{n!} L_{n+m+1}^{(D/2-1)}(Z^2)e^{-Z^2} .
\]

3.2.3 Lowering Relations of \(L_n^{(D/2-1)}(Z^2)e^{-Z^2}\)

In the previous section, the effect of differentiating NC\(\mu\)-Wavelets was shown to produce a function with higher orders of polynomials. In this section, a special differential relationship is derived which takes a NC\(\mu\)-Wavelet into one with a lower order polynomial. This will thus provide a lowering relation for the NC\(\mu\)-Wavelets.

Postulate that there exists a lowering relation of the form

\[
\left( \alpha \nabla \frac{\partial}{\partial Z} + \beta Z \right) L_n^{(D/2-1)}(Z^2)e^{-Z^2} = \gamma \frac{Z}{2} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} ,
\]

where \(\alpha, \beta,\) and \(\gamma\) are numbers. To determine these numbers, first look at the effect of

\[
\alpha \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1)}(Z^2)e^{-Z^2} = \alpha \left[ \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1)}(Z^2) \right] e^{-Z^2} + \alpha L_n^{(D/2-1)}(Z^2) \left[ \nabla \frac{\partial}{\partial Z} e^{-Z^2} \right] .
\]

Using the expression for the gradient of the \(L_n^{(D/2-1)}(Z^2)\) polynomial (eq. 3.43), gives

\[
\alpha \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1)}(Z^2)e^{-Z^2} = -2\alpha L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} - 2\alpha Z L_n^{(D/2-1)}(Z^2)e^{-Z^2} .
\]
Putting this result back into the left hand side of equation 3.100 gives

\[
\left( \alpha \frac{\nabla}{\nabla} + \beta \frac{\nabla}{\nabla} \right) L_n^{(D/2-1)}(Z^2)e^{-Z^2} \\
= -2\alpha \frac{\nabla}{\nabla} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} - 2\alpha \frac{\nabla}{\nabla} L_{n}^{(D/2-1)}(Z^2)e^{-Z^2} + \beta \frac{\nabla}{\nabla} L_{n}^{(D/2-1)}(Z^2)e^{-Z^2} \quad (3.103)
\]

In order to get this expression into the desired form (e.g. eq. 3.100) set \( \beta = 2\alpha \), giving

\[
\left( \alpha \frac{\nabla}{\nabla} + \beta \frac{\nabla}{\nabla} \right) L_n^{(D/2-1)}(Z^2)e^{-Z^2} \\
= -2\alpha \frac{\nabla}{\nabla} I_{n-1}^{(D/2)}(Z^2)e^{-Z^2} - 2\alpha \frac{\nabla}{\nabla} L_{n}^{(D/2-1)}(Z^2)e^{-Z^2} + 2\alpha \frac{\nabla}{\nabla} L_{n}^{(D/2-1)}(Z^2)e^{-Z^2} \quad (3.104a)
\]

\[
= -2\alpha \frac{\nabla}{\nabla} I_{n-1}^{(D/2)}(Z^2)e^{-Z^2} \quad (3.104b)
\]

Choosing the convention \( \alpha = -1/2 \) makes \( \gamma = 1 \) and thus the lowering of the \( l = 0 \) NC\( \mu \)-Wavelet is

\[
\left( -\frac{1}{2} \frac{\nabla}{\nabla} - \frac{\nabla}{\nabla} \right) L_n^{(D/2-1)}(Z^2)e^{-Z^2} = -\frac{\nabla}{\nabla} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} \quad (3.105)
\]

where for obvious reasons \( -\frac{1}{2} \frac{\nabla}{\nabla} - \frac{\nabla}{\nabla} \) will be known as the lowering operator.

Now consider the effect of a second application of the lowering operator to the \( l = 0 \) NC\( \mu \)-Wavelet. The result is

\[
\left( -\frac{1}{2} \frac{\nabla}{\nabla} - \frac{\nabla}{\nabla} \right)^2 L_n^{(D/2-1)}(Z^2)e^{-Z^2} = \left( -\frac{1}{2} \frac{\nabla}{\nabla} - \frac{\nabla}{\nabla} \right) \cdot \frac{\nabla}{\nabla} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} \quad (3.106a)
\]

\[
= -\frac{1}{2} \frac{\nabla}{\nabla} \cdot \left\{ \frac{\nabla}{\nabla} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} \right\} - Z^2 L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} \quad (3.106b)
\]

To evaluate this expression, it is best to tackle it part by part. Start by looking at the first term on the
right hand side separately, which by explicit differentiation equals

\[-\frac{1}{2} \frac{\nabla}{\nabla Z} \left[ Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right] = -\frac{1}{2} \left\{ \frac{\nabla}{\nabla Z} \left[ Z L_n^{(D/2)}(Z^2) \right] \left( Z e^{-Z^2} \right) \right\} + \frac{1}{2} \left\{ \nabla Z e^{-Z^2} \right\} \right] \]

(3.107)

Part (i) of this expression can be simplified by using equation, 3.83, as shown by

\[-\frac{1}{2} \left\{ \frac{\nabla}{\nabla Z} \left[ Z L_n^{(D/2)}(Z^2) \right] \left( Z e^{-Z^2} \right) \right\} = -\frac{1}{2} \left\{ 2(n - 1 + \frac{D}{2}) L_n^{(D/2-1)} e^{-Z^2} \right\} \]  

(3.108)

For part (ii) the gradient of the Gaussian can be computed to give

\[-\frac{1}{2} \frac{\nabla}{\nabla Z} \left[ Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right] = -\frac{1}{2} \nabla Z \left\{ Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} \]  

(3.109a)

\[-= Z^2 L_n^{(D/2)}(Z^2)e^{-Z^2}. \]  

(3.109b)

Putting these results back into equation 3.107 gives

\[-\frac{1}{2} \nabla Z \left[ Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right] = - \left( n - 1 + \frac{D}{2} \right) L_n^{(D/2-1)} e^{-Z^2} + Z^2 L_n^{(D/2)}(Z^2)e^{-Z^2}. \]  

(3.110)

Substitute this back into equation 3.106b yields

\[\left( -\frac{1}{2} \nabla Z - Z \right)^2 L_n^{(D/2-1)}(Z^2)e^{-Z^2} = - \left( n - 1 + \frac{D}{2} \right) L_n^{(D/2-1)} e^{-Z^2} + Z^2 L_n^{(D/2)}(Z^2)e^{-Z^2} \]  

(3.111a)

\[= - \left( n - 1 + \frac{D}{2} \right) L_n^{(D/2-1)} e^{-Z^2} \]  

(3.111b)

The second lowering of the \( l = 0 \) NC\( \mu \)-Wavelet is thus

\[\left( -\frac{1}{2} \nabla Z - Z \right)^2 L_n^{(D/2-1)}(Z^2)e^{-Z^2} = - \left( n - 1 + \frac{D}{2} \right) L_n^{(D/2-1)} e^{-Z^2}, \]  

(3.112)
and as a side result, the expression for the first lowering of the case \( I = 1 \) is seen to be

\[
\left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right) \cdot \left\{ \overrightarrow{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = - \left( n + \frac{D}{2} \right) L_n^{(D/2-1)}e^{-Z^2}.
\] (3.113)

Examining the effect of applying a second lowering operator to the \( I = 1 \) case, reveals that

\[
\left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^2 \left\{ \overrightarrow{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = - \left( n + \frac{D}{2} \right) \left\{ \left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right) L_n^{(D/2-1)}e^{-Z^2} \right\}.
\] (3.114)

which is equivalent to the first lowering of the \( I = 0 \) case multiplied by \(- (n + \frac{D}{2})\). Using equation 3.105 yields the second lowering of the \( I = 0 \) NC\( \mu \)-Wavelet as

\[
\left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^2 \left\{ \overrightarrow{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = - \left( n + \frac{D}{2} \right) \overrightarrow{Z} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2}.
\] (3.115)

With these results the general \( 2m \) lowerings can be determined. First consider the \( I = 0 \) case. Start by rewriting the \( 2m \) lowering as

\[
\left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^{2m} L_n^{(D/2-1)}(Z^2)e^{-Z^2} = \left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^{2m-2} \left\{ \left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^2 L_n^{(D/2-1)}(Z^2)e^{-Z^2} \right\}.
\] (3.116)

The quantity in the \{ \cdots \} brackets is given by equation 3.112, yielding

\[
\left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^{2m} L_n^{(D/2-1)}(Z^2)e^{-Z^2} = - \left( n + \frac{D}{2} \right) \left( -\frac{1}{2} \nabla_Z - \overrightarrow{Z} \right)^{2m-2} \left\{ L_{n-1}^{(D/2-1)}(Z^2)e^{-Z^2} \right\}.
\] (3.117)
Repeating this process,

\[
\begin{align*}
&= -\left(n + \frac{D}{2}\right) \left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m-4} \left\{\left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2} L_{n-1}^{(D/2-1)}(Z^2)e^{-Z^2}\right\} \\
&= (-1)^2 \left(n + \frac{D}{2}\right) \left(n - 1 + \frac{D}{2}\right) \left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m-6} \left\{\left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2} L_{n-2}^{(D/2-1)}(Z^2)e^{-Z^2}\right\}
\end{align*}
\] (3.118a)

allows the \(m\)th step to be deduced as

\[
(-1)^{2m} \frac{(n + \frac{D}{2})!}{(n - m - 1 + \frac{D}{2})!} L_{n-m}^{(D/2-1)}(Z^2)e^{-Z^2}.
\] (3.118b)

The \(2m\)th lowering of the \(l = 0\) NC\(\mu\)-Wavelet is thus

\[
\left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m} L_{n}^{(D/2-1)}(Z^2)e^{-Z^2} = (-1)^{2m} \frac{\Gamma(n+D/2+1)}{\Gamma(n-m+D/2)} L_{n-m}^{(D/2-1)}(Z^2)e^{-Z^2}.
\] (3.120)

It should be kept in mind \(L_{n-m}^{(D/2-1)} = 0\) for all positive integer values of \(j\). The \(l = 1\) case can be found by repeating the procedure,

\[
\begin{align*}
&= \left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m} \left[\frac{Z L_{n}^{(D/2)}(Z^2)e^{-Z^2}}{Z L_{n}^{(D/2)}(Z^2)e^{-Z^2}}\right] \\
&= \left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m-2} \left\{\left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2}\right\} \\
&= -\left(n + \frac{D}{2}\right) \left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2m-4} \left\{\left(-\frac{1}{2}, \frac{\partial}{\partial z} - \frac{1}{Z}\right)^{2} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2}\right\}
\end{align*}
\] (3.121a-b-c)
The $2m^{th}$ lowering of the $l = 1$ NC$_\mu$-Wavelet is thus

\[
\left(\frac{-1}{2} \nabla Z - \bar{Z}\right)^{2m} \left\{ Z L_n^{(D/2)} (Z^2) e^{-Z^2} \right\} = (-1)^{2m} \frac{\Gamma(n+D/2+1)}{\Gamma(n-m+D/2)} Z L_{n-m}^{(D/2)} (Z^2) e^{-Z^2}.
\] (3.122)

Lastly the $(2m + 1)^{th}$ lowerings can be found. Again start with the $l = 0$ case. Separate the $(2m + 1)^{th}$ lowering into

\[
\left(\frac{-1}{2} \nabla Z - \bar{Z}\right)^{2m+1} L_n^{(D/2-1)} (Z^2) e^{-Z^2} = \left(\frac{-1}{2} \nabla Z - \bar{Z}\right)^{2m} \left\{ \left(\frac{-1}{2} \nabla Z - \bar{Z}\right) L_n^{(D/2-1)} (Z^2) e^{-Z^2} \right\}.
\] (3.123)

The quantity in the bracket is given by equation 3.105, that is

\[
\left(\frac{-1}{2} \nabla Z - \bar{Z}\right)^{2m} \left\{ Z L_{n-1}^{(D/2)} (Z^2) e^{-Z^2} \right\}
\] (3.124)

which by equation 3.122 is

\[
(-1)^m \frac{(n-1+D/2)!}{(n-m+D/2)!} Z L_{n-m-1}^{(D/2)} (Z^2) e^{-Z^2}.
\] (3.125)

The $(2m + 1)^{th}$ lowering of the $l = 0$ NC$_\mu$-Wavelet is thus

\[
\left(\frac{-1}{2} \nabla Z - \bar{Z}\right)^{2m+1} L_n^{(D/2-1)} (Z^2) e^{-Z^2} = (-1)^{2m} \frac{\Gamma(n+D/2)}{\Gamma(n-m+D/2)} Z L_{n-m-1}^{(D/2)} (Z^2) e^{-Z^2}.
\] (3.126)
Repeating the process for the \( l = 1 \) case,

\[
\left( -\frac{1}{2} \nabla_Z - \overline{Z} \right)^{2m+1} \left[ \overline{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right]
\]

\[
= \left( -\frac{1}{2} \nabla_Z - \overline{Z} \right)^{2m+1} \left\{ \left( -\frac{1}{2} \nabla_Z - \overline{Z} \right) \cdot \{ \overline{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \} \right\}
\]

\[
= \left( -\frac{1}{2} \nabla_Z - \overline{Z} \right)^{2m+1} \left\{ - \left( n + \frac{D}{2} \right) L_n^{(D/2-1)} e^{-Z^2} \right\}
\]

\[
= - \left( n + \frac{D}{2} \right)^{2m+1} \left[ \left( -\frac{1}{2} \nabla_Z - \overline{Z} \right)^{2m} L_n^{(D/2-1)} e^{-Z^2} \right]
\]

\[
yields \text{the } (2m+1)^{th} \text{ lowering of the } l = 1 \text{ NC} \mu \text{-Wavelet as}
\]

\[
\left( -\frac{1}{2} \nabla_Z - \overline{Z} \right)^{2m+1} \left[ \overline{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \right] = (-1)^{2m+1} \left( n + \frac{D}{2} \right)^{\frac{(n+D/2+1)!}{(n-m-1+D/2)!}} L_n^{(D/2-1)} e^{-Z^2}.
\]

\[
(3.128)
\]

### 3.3 The Ladder Operators of the NC\( \mu \)-Wavelets

In order to gain physical insight, it is instructive to examine NC\( \mu \)-Wavelets using the operator formalism. This discussion represents the non-Cartesian generalization of reference [55], which examined the special case of one dimension. Consider an operator\(^5\) \( \mathbf{P} \) that when applied to the \( n^{th} \) NC\( \mu \)-Wavelet results in the \( (n+1)^{th} \) NC\( \mu \)-Wavelet multiplied by a constant. This process is symbolized by

\[
\mathbf{P} \phi_n^{(D/2-1+l)}(\overline{Z}) = P_{nl} \phi_{n+1}^{(D/2-1+l)}(\overline{Z}),
\]

\[
(3.129)
\]

where \( \phi_n^{(D/2-1+l)} \) is the NC\( \mu \)-Wavelet and \( P_{nl} \) is the constant that may depend on \( n, l, D, \) or other parameters. When such an operator \( \mathbf{P} \) does not itself depend on \( n \), it is known as a raising operator. Similarly, there is a lowering operator \( \Delta \) independent of \( n \), that when applied to the \( n^{th} \) NC\( \mu \)-Wavelet

---

\(^5\)the symbol \( \mathbf{P} \) used here is the capital Greek letter \( \rho \) "rho."
produces
\[ \Lambda \phi_n^{(D/2-1+l)}(\overrightarrow{Z}) = \Lambda_n \phi_{n-1}^{(D/2-1+l)}(\overrightarrow{Z}), \]  
(3.130)

where \( \Lambda_n \) is a multiplicative constant. Together raising and lowering operators are known as ladder operators as they step an index up or down. It should be noted that NC\( \mu \)-Wavelets have another index, \( l \), which is also subject to raising and lowering; however, some changes in the \( l \) index require the \( n \) index also to be changed. This can be seen by comparing the polynomial degree of the two types of NC\( \mu \)-Wavelets. The \((n^{th}, l = 1)\) NC\( \mu \)-Wavelet
\[ \overrightarrow{\phi}_n^{(D/2)}(\overrightarrow{Z}) = \overrightarrow{Z} L_n^{(D/2)}(Z^2)e^{-Z^2} \]  
(3.131)
is one degree higher than the \((n^{th}, l = 0)\) NC\( \mu \)-Wavelet
\[ \phi_n^{(D/2-1)}(\overrightarrow{Z}) = L_n^{(D/2-1)}(Z^2)e^{-Z^2}, \]  
(3.132)
but is one degree lower than the \(((n+1)^{th}, l = 0)\) NC\( \mu \)-Wavelet
\[ \phi_{n+1}^{(D/2-1)}(\overrightarrow{Z}) = L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2}. \]  
(3.133)

With this in mind, there is another raising operator, \( \overrightarrow{\rho} \), such that
\[ \overrightarrow{\rho} \phi_n^{(D/2)}(\overrightarrow{Z}) = \rho_n \phi_{n+1}^{(D/2-1)}(\overrightarrow{Z}), \]  
(3.134a)
\[ \overrightarrow{\rho} \phi_n^{(D/2-1)}(\overrightarrow{Z}) = \rho_n \phi_{n}^{(D/2)}(\overrightarrow{Z}), \]  
(3.134b)
and lowering operator, $\overrightarrow{\lambda}$, such that

$$\overrightarrow{\lambda} \phi_n^{(D/2)}(\overrightarrow{Z}) = \lambda_{n1} \phi_{n-1}^{(D/2)}(\overrightarrow{Z}) \quad (3.135a)$$

$$\overrightarrow{\lambda} \phi_n^{(D/2-1)}(\overrightarrow{Z}) = \lambda_{n0} \phi_{n-1}^{(D/2)}(\overrightarrow{Z}) \quad (3.135b)$$

where $\rho_{nl}$ and $\lambda_{nl}$ are the multiplicative constants. Now consider the applications of the two $\overrightarrow{\rho}$ raising operators, shown here

$$\overrightarrow{\rho} \cdot \overrightarrow{\rho} \phi_n^{(D/2-1)}(\overrightarrow{Z}) = \rho_{n0} \overrightarrow{\rho} \phi_n^{(D/2)}(\overrightarrow{Z}) \quad (3.136a)$$

$$= \rho_{n0} \rho_{n1} \phi_{n+1}^{(D/2-1)}(\overrightarrow{Z}) \quad (3.136b)$$

and here

$$\overrightarrow{\rho} \cdot \overrightarrow{\rho} \phi_n^{(D/2)}(\overrightarrow{Z}) = \rho_{n1} \overrightarrow{\rho} \phi_{n+1}^{(D/2-1)}(\overrightarrow{Z}) \quad (3.137a)$$

$$= \rho_{n1} \rho_{n+1} \phi_{n+1}^{(D/2)}(\overrightarrow{Z}) \quad (3.137b)$$

Comparing with equation 3.129 shows that

$$\overrightarrow{\rho} \cdot \overrightarrow{\rho} \equiv P \quad (3.138)$$

and

$$\rho_{n0} \rho_{n1} \equiv P_n \quad (3.139a)$$

$$\rho_{(n+1)0} \rho_{n1} \equiv P_{n1} \quad (3.139b)$$

Similarly, it can be seen that

$$\overrightarrow{\lambda} \cdot \overrightarrow{\lambda} \equiv \Lambda \quad (3.140)$$
and

$$\lambda_{(n-1) \lambda_{n0}} \equiv \lambda_{n0} \quad (3.141a)$$

$$\lambda_{n0} \lambda_{n1} \equiv \lambda_{n1} \quad (3.141b)$$

From this it can be concluded that $\vec{p}$ and $\vec{A}$ are the fundamental ladder operators for NC$\mu$-Wavelets.

It is useful to look at a few of the properties of these ladder operators. Consider the effect of applying the product $\vec{p} \cdot \vec{A}$ to the NC$\mu$-Wavelets. The result is

$$\vec{p} \cdot \vec{A} \phi_{n}^{(D/2)}(Z) = \vec{p} \cdot \{ \vec{A} \cdot \phi_{n}^{(D/2)}(Z) \} \quad (3.142a)$$

$$= \lambda_{n1} \vec{p} \phi_{n}^{(D/2-1)}(Z) \quad (3.142b)$$

$$= \lambda_{n1} \rho_{n0} \phi_{n}^{(D/2)}(Z) \quad (3.142c)$$

and

$$\vec{p} \cdot \vec{A} \phi_{n}^{(D/2-1)}(Z) = \vec{p} \cdot \{ \vec{A} \phi_{n}^{(D/2-1)}(Z) \} \quad (3.143a)$$

$$= \lambda_{n0} \vec{p} \phi_{n-1}^{(D/2)}(Z) \quad (3.143b)$$

$$= \lambda_{n0} \rho_{n1} \phi_{n}^{(D/2-1)}(Z) \quad (3.143c)$$

The effect is thus the original NC$\mu$-Wavelet multiplied by a constant. From this it can be concluded that NC$\mu$-Wavelets are eigenstates of the operator $\vec{p} \cdot \vec{A}$ with the eigenvalues $\lambda_{n1} \rho_{n0}$ and $\lambda_{n0} \rho_{n1}$ for the $(n, l = 1)$ and $(n, l = 0)$ NC$\mu$-Wavelets respectively. NC$\mu$-Wavelet are also eigenstates of the
product $\vec{x} \cdot \vec{p}$, but, as can be seen by

$$\vec{x} \cdot \vec{p} \psi_n^{(D/2)}(\vec{Z}) = \lambda_n \left\{ \vec{p} \psi_n^{(D/2)}(\vec{Z}) \right\}$$

(3.144a)

$$= C_n \lambda_n \phi_{n+1}^{(D/2-1)}(Z^2)$$

(3.144b)

$$= C_n \lambda_n \phi_{n}^{(D/2)}(\vec{Z})$$

(3.144c)

with different eigenvalues. It is also true, by the superposition principle [4], that the NC$\mu$-Wavelets are eigenstates of any linear combination of $\vec{p} \cdot \vec{x}$ and $\vec{x} \cdot \vec{p}$. This point will be returned to later. Now consider the effect of applying the lowering operator to the lowest $l = 0$ function, that is the $n = 0$ one. The result is

$$\vec{x} \phi_0^{(D/2-1)}(\vec{Z}) = \lambda_0 \phi_{-1}^{(D/2)}(\vec{Z})$$

(3.146)

but since

$$\phi_{-1}^{(D/2)}(\vec{Z}) = L_{-1}^{(D/2)}(Z^2) e^{-Z^2} = 0$$

(3.147)

the lowering operator is said to annihilate the $(n = 0, l = 0)$ NC$\mu$-Wavelet. This is just a reflection of the fact demonstrated in chapter 2 that $\phi_0^{(D/2-1)}(\vec{Z})$ is a minimum uncertainty state. This does not mean, however, that $\vec{x}$ is the same annihilation operator used in that chapter (eq. 2.48, p20). It should also be noted that

$$\Lambda \phi_0^{(D/2-1)}(\vec{Z}) = \Lambda_{00} \phi_{-1}^{(D/2-1)}(\vec{Z}) = 0$$

(3.148)
that is, the lowering operator \( A \) also annihilates the \((n = 0, l = 0)\) NC\(\mu\)-Wavelet. Now considering the application of \( \nabla \) to the lowest \( l = 1 \) NC\(\mu\)-Wavelet. The result of that operation is

\[
\nabla \cdot \phi^{(D/2)}_0 (\vec{Z}) = \lambda_{01} \phi^{(D/2-1)}_0 (\vec{Z}) ,
\]

which is nonvanishing, but

\[
A \phi^{(D/2)}_0 (\vec{Z}) = \Lambda_{01} \phi^{(D/2)}_{-1} (\vec{Z}) = 0 .
\]

The lowering operator \( \Lambda \) is thus the annihilation operator of both \( \phi^{(D/2-1)}_0 (\vec{Z}) \) and \( \phi^{(D/2)}_0 (\vec{Z}) \).

Further understanding of these ladder operators can be made by equating them with the results of the previous section. When the expressions for the raising of the NC\(\mu\)-Wavelets (eq. 3.134) is compared to the effect of the gradient (section 3.2.2) the raising operator is revealed to be

\[
\vec{\nabla} \Rightarrow -\frac{1}{2} \vec{\nabla} \nabla ,
\]

in the position representation. The corresponding multiplicative numbers are

\[
\begin{align*}
    \rho_{n0} &= 1 \\
    \rho_{n1} &= -(n + 1)
\end{align*}
\]

Likewise, comparing the lowering operator of equation 3.135 to the lowering relations of section 3.2.3 confirms the lowering operator to be

\[
\nabla \Rightarrow \left( -\frac{1}{2} \nabla \nabla - \nabla \right) ,
\]
in the position domain. The corresponding multiplicative numbers are

\[
\begin{align*}
\lambda_{n0} &= 1 \\
\lambda_{n1} &= -(n + \frac{D}{2})
\end{align*}
\] (3.154)

It is instructive to write the NC\(\lambda\)-Wavelet ladder operators in their abstract forms. When the raising operator \(\check{\rho}\) is compared to the (scaled) \(D\)-dimensional momentum operator in the position domain,

\[\check{\mathbf{p}} \Rightarrow -i\nabla_{\mathbf{r}},\] (3.155)

the abstract form of the operator is clearly seen to be

\[
\check{\rho} \equiv -\frac{1}{2} \check{\mathbf{p}}.
\] (3.156)

The \(\check{\rho}\) raising operator is thus related to momentum. By taking the product \(\check{\rho} \cdot \check{\rho}\), the \(\mathbf{P}\) operator is seen to be

\[
\mathbf{P} \equiv -\frac{1}{4} \check{\mathbf{p}} \cdot \check{\mathbf{p}},
\] (3.157)

which relates it to the kinetic energy. The corresponding multiplicative numbers are

\[
\begin{align*}
P_{n0} &= \rho_{n0}\rho_{n1} = -(n + 1) \quad (3.158a) \\
P_{n1} &= \rho_{n1}\rho_{(n+1),0} = -(n + 1) \quad (3.158b) \\
P_{nl} &= -(n + 1),
\end{align*}
\] (3.159)

meaning that it is independent of \(l\). The lowering operator likewise can be converted to its abstract
form,

$$\bar{x} = \left( -\frac{1}{2} \nabla \cdot \bar{z} - \bar{z} \right)$$  \hspace{1cm} (3.160a)

$$= \left( -\frac{1}{2} \bar{y} - \bar{z} \right)$$  \hspace{1cm} (3.160b)

yielding

$$\bar{x} \equiv -\left( \bar{z} + \frac{1}{2} \bar{y} \right)$$  \hspace{1cm} (3.161)

It is important to note that this lowering operator is distinctly different than with the harmonic oscillator lowering operator (appendix 3D),

$$\bar{\alpha} = \frac{1}{2} \left( \bar{z} + i\bar{y} \right)$$  \hspace{1cm} (3.162)

The relation between the two is

$$\bar{\alpha} = -\frac{1}{2} \left( \bar{x} + \bar{\rho} \right)$$  \hspace{1cm} (3.163)

The relation with the corresponding raising operator is simply the adjoint

$$\bar{\alpha}^\dagger = -\frac{1}{2} \left( \bar{x}^\dagger + \bar{\rho}^\dagger \right)$$  \hspace{1cm} (3.164)

Now consider the product $\bar{x} \cdot \bar{x} = \Lambda$. When multiplied out,

$$\Lambda = \bar{x} \cdot \bar{x}$$  \hspace{1cm} (3.165a)

$$= \left( \bar{z} + \frac{1}{2} i\bar{y} \right) \cdot \left( \bar{z} + \frac{1}{2} i\bar{y} \right)$$  \hspace{1cm} (3.165b)

$$= \left( \bar{z} \cdot \bar{z} + i\frac{1}{2} \bar{z} \cdot \bar{y} + i\frac{1}{2} \bar{y} \cdot \bar{z} - \frac{1}{4} \bar{y} \cdot \bar{y} \right)$$  \hspace{1cm} (3.165c)

and using $\bar{y} \cdot \bar{z} = D + \bar{z} \cdot \bar{y}$ results in

$$\Lambda = \left( \bar{z} \cdot \bar{z} + i\bar{z} \cdot \bar{y} + i\frac{1}{2} I - \frac{1}{4} \bar{y} \cdot \bar{y} \right)$$  \hspace{1cm} (3.165d)
The corresponding multiplicative numbers are

\[
\begin{align*}
\Lambda_{n0} &= -(n + \frac{D}{2} - 1), \\
\Lambda_{n1} &= -(n + \frac{D}{2})
\end{align*}
\tag{3.166}
\]

which, unlike the \(P_{nl}\) case, bears a \(l\) dependence.

It will be useful to establish the physical quantities momentum, position, and energy in terms of the ladder operators. Momentum is found by a trivial reversal of equation 3.156, that is

\[
\overrightarrow{\mathbf{r}} \equiv \overrightarrow{\mathbf{r}}
\tag{3.167}
\]

To find position consider the effect of the operator \(\left(\overrightarrow{\rho} - \overrightarrow{\mathbf{x}}\right)\). When applied to \(l = 0\), the result is

\[
\begin{align*}
\left(\overrightarrow{\rho} - \overrightarrow{\mathbf{x}}\right) \phi_{n}^{(D/2-1)}(Z) &= \overrightarrow{\rho} \phi_{n}^{(D/2-1)}(Z) - \overrightarrow{\mathbf{x}} \phi_{n}^{(D/2-1)}(Z) \\
&= \rho_{n0} \phi_{n}^{(D/2)}(Z) - \lambda_{n0} \phi_{n-1}^{(D/2)}(Z^2) + \\
&= \overrightarrow{Z} L_{n}^{(D/2)}(Z^2)e^{-Z^2} - \overrightarrow{Z} L_{n-1}^{(D/2)}(Z^2)e^{-Z^2} + \\
&= \overrightarrow{Z} \left[ L_{n}^{(D/2)}(Z^2) - L_{n-1}^{(D/2)}(Z^2) \right] e^{-Z^2}.
\end{align*}
\tag{3.168}
\]

Using the recursion \(L_{n}^{(D/2)} - L_{n-1}^{(D/2)} = L_{n}^{(D/2-1)}\) (eq. 3.35) yields

\[
\left(\overrightarrow{\rho} - \overrightarrow{\mathbf{x}}\right) \phi_{n}^{(D/2-1)}(Z) = \overrightarrow{Z} \phi_{n}^{(D/2-1)}(Z) .
\tag{3.172}
\]

Position in terms of raising and lowering operator is therefore

\[
\overrightarrow{Z} \equiv \left(\overrightarrow{\rho} - \overrightarrow{\mathbf{x}}\right).
\tag{3.173}
\]

To find energy, first recall the claim that the NC\(\mu\)-Wavelets are eigenstates of any linear combination
of $\overrightarrow{p} \cdot \overrightarrow{A}$ and $\overrightarrow{A} \cdot \overrightarrow{p}$. It can easily be demonstrated that the same is true of any combination of $PA$ and $\Delta P$, as shown by

$$PA\phi_n^{(D/2-1+i)}(\overrightarrow{Z}) = P\left\{A\phi_n^{(D/2-1+i)}(\overrightarrow{Z})\right\}$$

$$= A_n P\left\{\phi_{n-1}^{(D/2-1+i)}(\overrightarrow{Z})\right\}$$

$$= A_n P_{(n-1)}\phi_n^{(D/2-1+i)}(\overrightarrow{Z})$$

(3.174a)

(3.174b)

(3.174c)

$$\Delta P\phi_n^{(D/2-1+i)}(\overrightarrow{Z}) = \Delta \left\{P\phi_n^{(D/2-1+i)}(\overrightarrow{Z})\right\}$$

$$= P_{n1}\Delta \left\{\phi_{n+1}^{(D/2-1+i)}(\overrightarrow{Z})\right\}$$

$$= P_{n1}\Lambda_{(n+1)}\phi_n^{(D/2-1+i)}(\overrightarrow{Z}) .$$

(3.175a)

(3.175b)

(3.175c)

An inspired choice is

$$\Delta P - PA = [\Lambda, P] ,$$

(3.176)

where $[,]$ is the commutator. When applied to $\phi_n^{(D/2-1+i)}(\overrightarrow{Z})$ the result is

$$[\Lambda, P]\phi_n^{(D/2-1+i)}(\overrightarrow{Z}) = \Delta P\phi_n^{(D/2-1+i)}(Z^2) - PA\phi_n^{(D/2-1+i)}(Z^2)$$

$$= (P_{n1}\Lambda_{(n+1)} - A_n P_{(n-1)}\phi_n^{(D/2-1+i)}(Z^2) .$$

(3.177a)

(3.177b)

Resolving the eigenvalues gives

$$P_{n0}\Lambda_{(n+1)0} - A_n P_{(n-1)0} = (n + 1) \left( n + D \over 2 \right) - \left( n + D \over 2 - 1 \right) n$$

$$= n^2 + \frac{D}{2} n + \frac{D}{2} - n^2 - n^2 \frac{D}{2} + n$$

$$= \frac{D}{2} + 2n .$$

(3.178a)

(3.178b)

(3.178c)
and

\[ P_{n+1}(n+1) - \Lambda_{n}P_{n-1} = (n+1) \left( n + \frac{D}{2} + 1 \right) - \left( n + \frac{D}{2} \right) n \]

\[ = n^2 + n\frac{D}{2} + n + n + \frac{D}{2} + 1 - n^2 - n\frac{D}{2} \]

\[ = (2n+1) + \frac{D}{2}. \]  

(3.179a)

(3.179b)

(3.179c)

To put these results in a more recognizable form, let

\[ H = [\Lambda, P] \]  

(3.180)

and \( H_n = P_{n+1} - \Lambda_{n}P_{n-1} \), yielding

\[
\begin{align*}
H_{n0} &= 2n + \frac{D}{2} \\
H_{n1} &= (2n+1) + \frac{D}{2} \\
H_{nl} &= (2n + l) + \frac{D}{2}
\end{align*}
\]

(3.181)

 Readers well versed in quantum mechanics will easily recognize this as the energy eigenvalues (even and odd parity respectively) of the \( D \) dimensional (isotropic) harmonic oscillator\(^6\); however, one can not further conclude that the spectra of the \( l = 0,1 \) NC\( \mu \)-Wavelets are identical to the harmonic oscillator. This is due to the fact that the degeneracies of the eigenvalues have not been taken into consideration. For example, when \( D = 3 \) there are 6 harmonic oscillator states with the energy of \( \frac{11}{2} \) but only 1 NC\( \mu \)-Wavelet (of the type discussed here) corresponding to that energy value. The \( l = 0,1 \) NC\( \mu \)-Wavelets can only account for states that transform under rotation as scalars and vectors respectively. This means for \( D \geq 3 \) the set of \( l = 0,1 \) NC\( \mu \)-Wavelets are incomplete. The answer to this dilemma is that there exist NC\( \mu \)-Wavelets for higher values of \( l \). Since they do not find application in this work, their discussion is deferred to future publications.

\(^6\)Note that some text use a different \( n' \) which is equal to \( n + l \) or \( n + l/2 \).
Appendix 3A: Associated Laguerre Polynomials

The purpose of this appendix is to provide a quick reference to the expressions for associated Laguerre polynomials (which are also known as Generalized Laguerre polynomials). The reader is referred to [2][101][102] for detailed discussions. Attention should be paid to the conventions used here as some text define the polynomials differently\(^7\).

Definition

Associated Laguerre polynomials can be defined in terms of a recursion relation,

\[(n + 1) L_{n+1}^\alpha(x) = (2n - x + \alpha + 1) L_n^\alpha(x) - (n + \alpha) L_{n-1}^\alpha(x), \quad (3A.1)\]

along with the specification of the first two polynomials

\[L_0^\alpha(x) = 0 \]
\[L_1^\alpha(x) = 1 \quad \text{for } \alpha = 0 \]
\[L_0^\alpha(x) = 1 \quad \text{for } \alpha > 0 \]

Generator Expression

\[L_n^\alpha(x) = \frac{1}{n!} x^{-\alpha} e^{x} \frac{d^n}{dx^n} \left[ x^{n+\alpha} e^{-x} \right] \quad (3A.3)\]

First Few Polynomials

\[L_0^\alpha(x) = 0 \]
\[L_1^\alpha(x) = 1 \]
\[L_2^\alpha(x) = -x + (\alpha + 1) \]
\[L_3^\alpha(x) = \frac{1}{2} \left[ x^2 - 2(\alpha + 2)x + (\alpha + 1)(\alpha + 2) \right] \]
\[L_4^\alpha(x) = \frac{1}{6} \left[ -x^3 + 3(\alpha + 4)x^2 - 3(\alpha + 2)(\alpha + 3)x + (\alpha + 1)(\alpha + 2)(\alpha + 3) \right] \]

\(^7\)for example Schaum's Outline Series: Mathematical Handbook of Formulas and Tables, ed. by Murray R. Spiegel
Recursion Relationships

\[(n + 1) L_n^{\alpha+1}(x) = (2n - x + \alpha + 1) L_n^{\alpha}(x) - (n + \alpha) L_n^{\alpha-1}(x) \] \hspace{1cm} (3A.5)

\[L_n^{\alpha}(x) = L_n^{\alpha+1}(x) - L_{n-1}^{\alpha+1}(x) \] \hspace{1cm} (3A.6)

\[x L_n^{\alpha+1}(x) = (x - n) L_n^{\alpha}(x) - (n + \alpha) L_n^{\alpha-1}(x) \] \hspace{1cm} (3A.7)

\[x L_n^{\alpha+1}(x) = (n + \alpha + 1) L_n^{\alpha}(x) - (n + 1) L_{n+1}^{\alpha}(x) \] \hspace{1cm} (3A.8)

\[(n + \alpha) L_n^{\alpha-1}(x) = (n + 1) L_n^{\alpha}(x) - (n + 1 - x) L_n^{\alpha}(x) \] \hspace{1cm} (3A.9)

\[\sum_{j=0}^{n} L_j^{\alpha}(x) = L_n^{\alpha+1}(x) \] \hspace{1cm} (3A.10)

Derivative Relationship

\[\frac{d}{dx} L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x) \] \hspace{1cm} (3A.11)

Value at \(x = 0\)

\[L_n^{(\alpha)}(0) = \frac{\Gamma(n + \alpha + 1)}{\Gamma(n + 1)} \] \hspace{1cm} (3A.12)

Orthogonality

\[\int_0^\infty dx e^{-x} x^\alpha L_n^{(\alpha)}(x) L_n^{(\alpha)}(x) = \frac{\Gamma(n + \alpha + 1)}{\Gamma(n + 1)} \delta_{n,m} \] \hspace{1cm} (3A.13)

Note, this orthogonality is defined over the range \(x = [0, \infty)\) where \(\delta_{n,m}\) is the Kronecker delta and \(\Gamma(\cdot)\) is the gamma function.

Relation to Laguerre Polynomials

\[L_n^{(\alpha)}(x) = (-1)^n \frac{d^n}{dx^n} L_{n+\alpha}(x) \] \hspace{1cm} (3A.14)
Relation to Hermite Polynomials

\[ L_{n}^{(-1/2)}(x^2) = (-1)^n \frac{1}{n!} \frac{1}{2^n} H_{2n}(x) \]

\[ L_{n}^{(1/2)}(x^2) = (-1)^n \frac{1}{n!} \frac{1}{2^n} H_{2n+1}(x) \]  

(3A.15)
Appendix 3B: Proof of Recursion Relationship 3.39

It is the purpose of this appendix to prove the recursion relationship

\[ DL_n^{(D/2)}(Z^2) - 22^2 I_{n-1}^{(D/2+1)}(Z^2) = 2 \left( n + \frac{D}{2} \right) I_n^{(D/2-1)}(Z^2) \]  
\[ (3B.1) \]

First convert the second term on the left hand side by using recursion equation 3.37,

\[ -22^2 I_{n-1}^{(D/2+1)} = +2nI_n^{(D/2)} - 2 \left( n + \frac{D}{2} \right) I_{n-1}^{(D/2)} \]
\[ (3B.2) \]

yielding

\[ DL_n^{(D/2)} + \left( 2nL_n^{(D/2)} - 2 \left( n + \frac{D}{2} \right) L_n^{(D/2)} \right) \]
\[ DL_n^{(D/2)} + 2nL_n^{(D/2)} - 2 \left( n + \frac{D}{2} \right) L_n^{(D/2)} \]
\[ 2 \left( \frac{D}{2} + n \right) L_n^{(D/2)} - 2 \left( n + \frac{D}{2} \right) L_n^{(D/2)} \]
\[ 2 \left( \frac{D}{2} + n \right) \left\{ I_n^{(D/2)} - L_n^{(D/2)} \right\} \]
\[ (3B.3a) \]
\[ (3B.3b) \]
\[ (3B.3c) \]
\[ (3B.3d) \]

Now using recursion equation 3.35 results in

\[ L_n^{(D/2)} - L_n^{(D/2)} = L_n^{(D/2-1)}(r^2) \]
\[ (3B.4) \]

which shows the right hand side equals the left hand side,

\[ 2 \left( \frac{D}{2} + n \right) L_n^{(D/2-1)}(Z^2) = 2 \left( n + \frac{D}{2} \right) L_n^{(D/2-1)}(Z^2) \]
\[ (3B.5) \]
Appendix 3C: Proof of Recursion Relationship 3.40

The purpose of this appendix is to prove the recursion relations (eq. 3.40)

\[ Z^2 L_n^{(D/2+1)}(Z^2) - \frac{D}{2} L_n^{(D/2)}(Z^2) = -(n + 1) L_{n+1}^{(D/2-1)}(Z^2). \]  

(3C.1)

It should be noted they are not simple variations of those found in the chapter.

First the relation

\[ \nabla \frac{\partial}{\partial Z} \left\{ L_n^{(D/2-1+l)}(Z^2)e^{-Z^2} \right\} = -2 \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1+l+1)}(Z^2)e^{-Z^2} \]  

(3C.2)

needs to be proven for any integer \( l \geq 0 \) (see eq. 3.42 for the special cases \( l = 0 \) and \( l = 1 \)).

Differentiate the left hand side gives

\[
\begin{align*}
\left\{ \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1+l)}(Z^2)e^{-Z^2} \right\} &= \left\{ \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1+l)}(Z^2) \right\} e^{-Z^2} + L_n^{(D/2-1+l)}(Z^2) \left\{ \nabla \frac{\partial}{\partial Z} e^{-Z^2} \right\} \\
&= \left\{ \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1+l)}(Z^2) \right\} \left( \nabla \frac{\partial}{\partial Z} \right) \cdot Z^2 - 2 \nabla \frac{\partial}{\partial Z} L_n^{(D/2-1+l)}(Z^2)e^{-Z^2} \\
&= -2 \nabla \frac{\partial}{\partial Z} \left( L_{n-1}^{(D/2-1+l+1)}(Z^2) + L_n^{(D/2-1+l)}(Z^2) \right) e^{-Z^2}.
\end{align*}
\]  

(3C.3a)

(3C.3b)

Using the recursion

\[ L_n^\alpha = L_n^{\alpha+1} - L_{n-1}^{\alpha+1} \]  

(3C.4a)

\[ L_n^\alpha + L_{n-1}^{\alpha+1} = L_n^{\alpha+1}, \]  

(3C.4b)

yields

\[ \left( L_{n-1}^{(D/2-1+l+1)}(Z^2) + L_n^{(D/2-1+l)}(Z^2) \right) = L_n^{(D/2-1+l+1)}(Z^2). \]  

(3C.5)
The relation for any integer $I \geq 0$ is thus

$$\nabla_Z \left\{ L_n^{(D/2-1+I)}(Z^2)e^{-Z^2} \right\} = -2Z L_n^{(D/2-1+I+1)}(Z^2)e^{-Z^2}.$$  \hfill (3C.6)

Now consider

$$\frac{Z^2 L_n^{(D/2+1)}(Z^2)e^{-Z^2}}{\text{LHS (i)}} - \frac{D}{2} \frac{L_n^{(D/2)}(Z^2)e^{-Z^2}}{\text{LHS (ii)}} = -(n + 1) L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2}.$$  \hfill (3C.7)

which is 3C.1 multiplied by $e^{-Z^2}$. Start by using equation 3C.6 on part (i) to rewrite it as

$$Z^2 L_n^{(D/2+1)}(Z^2)e^{-Z^2} = \nabla_Z \left\{ Z L_n^{(D/2+1)}(Z^2)e^{-Z^2} \right\}$$  \hfill (3C.8a)

$$= \nabla_Z \left\{ -\frac{1}{2} \nabla_Z \left\{ L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} \right\}$$  \hfill (3C.8b)

$$= -\frac{1}{2} \nabla_Z \cdot \nabla_Z \left\{ L_n^{(D/2)}(Z^2)e^{-Z^2} \right\}.$$  \hfill (3C.8c)

Note that

$$\nabla_Z \cdot \left\{ \nabla_Z \psi \right\} = \nabla_Z \cdot \nabla_Z \psi + \nabla_Z \cdot \nabla_Z \left\{ \psi \right\}$$  \hfill (3C.9a)

$$= D\psi + \nabla_Z \cdot \nabla_Z \left\{ \psi \right\},$$  \hfill (3C.9b)

allows the LHS to be rewritten as

$$-\frac{1}{2} \left( \nabla_Z \cdot \nabla_Z + D \right) \left\{ L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = -\frac{1}{2} \nabla_Z \cdot \left\{ \nabla_Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right\}.$$  \hfill (3C.10)

Now use the generator expression for the quantity in the bracket,

$$-\frac{1}{2} \nabla_Z \cdot \left\{ \nabla_Z L_n^{(D/2)}(Z^2)e^{-Z^2} \right\} = -\frac{1}{2} \nabla_Z \cdot \left\{ -\frac{1}{2} \left( -\frac{1}{4} \right)^n \frac{1}{n!} \nabla_Z^{2n+1} e^{-Z^2} \right\}.$$  \hfill (3C.11)
yielding
\[ \frac{1}{4} \left( -\frac{1}{4} \right)^n \frac{1}{n!} \nabla^{2n+2} e^{-Z^2} \] for the LHS. \hfill (3C.12)

Now write the RHS in terms of the generator expression,
\[-(n+1) \left\{ L_{n+1}^{(D/2-1)}(Z^2)e^{-z^2} \right\} = -(n+1) \left\{ \left( -\frac{1}{4} \right)^{n+1} \frac{1}{(n+1)!} \nabla^{2n+2} e^{-Z^2} \right\} \] \hfill (3C.13)

yielding
\[ \frac{1}{4} \left( -\frac{1}{4} \right)^n \frac{1}{n!} \nabla^{2n+2} e^{-Z^2} \] for the RHS. \hfill (3C.14)

The RHS matches the LHS, therefore
\[
\begin{align*}
Z^2 L_n^{(D/2+1)}(Z^2)e^{-Z^2} - \frac{D}{2} L_n^{(D/2)}(Z^2)e^{-Z^2} &= -(n+1) L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2} \quad (3C.15a) \\
Z^2 L_n^{(D/2+1)}(Z^2)e^{-Z^2} e^{z^2} - \frac{D}{2} L_n^{(D/2)}(Z^2)e^{-Z^2} e^{z^2} &= -(n+1) L_{n+1}^{(D/2-1)}(Z^2)e^{-Z^2} e^{z^2} \quad (3C.15b)
\end{align*}
\]

\[
Z^2 L_n^{(D/2+1)}(Z^2) - \frac{D}{2} L_n^{(D/2)}(Z^2) = -(n+1) L_{n+1}^{(D/2-1)}(Z^2) \] \hfill (3C.16)
Appendix 3D: Ladder Operators of the D-Dimensional Isotropic Harmonic Oscillator

In this appendix some useful ladder operators of the D-dimensional isotropic harmonic oscillator are examined. Since only \( l = 0 \) and \( 1 \) are relevant to this chapter attention will be restricted to these cases.

The ladder operators of the radial part of the harmonic oscillator wavefunction are well-known (see [105] for example) but they are not in a form analogous to the ladder operators of the NC\(_\mu\)-Wavelets. The conversion, however, is rather simple and starts by considering the wavefunction in hyperpherical coordinates [105, eq. 2.1 with \( \lambda \rightarrow \frac{1}{2\sigma^2} \) and \( N \rightarrow D \)],

\[
\psi_{\ell m} (\vec{r}; D, \sigma) = \left( \frac{1}{2\sigma^2} \right)^{D/4} \left( \frac{(2n)!}{\Gamma(\frac{D}{2} + l + n)} \right)^{1/2} \left[ Y_{\ell m}(\Omega_D) \left( \frac{1}{\sqrt{2\sigma}} \right)^l \right] L_n^{D/2-1+l}(\frac{r^2}{2\sigma^2}) \exp\left(-\frac{r^2}{4\sigma^2}\right). \tag{3D.1}
\]

Rewrite the \( l = 0 \) and \( 1 \) cases in terms of irreducible Cartesian tensors [103][104] using

\[
Y_{\ell m} \Rightarrow \left( \frac{\Gamma(D/2)}{2\pi^{D/2}} \right)^{1/2}
\]

\[
Y_{1m} \left( \frac{1}{\sqrt{2\sigma}} \right) r \Rightarrow \left( \frac{\Gamma(D/2 + 1)}{\pi^{D/2}} \right)^{1/2} \left( \frac{\vec{r}}{\sqrt{2\sigma}} \right)
\]

(3D.2) (3D.3)

to give

\[
\psi_{n0} (\vec{r}; D, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/4} \left( \frac{(2n)!\Gamma(D/2)}{2\Gamma(\frac{D}{2} + n)} \right)^{1/2} L_n^{D/2-1}(\frac{r^2}{2\sigma^2}) \exp\left(-\frac{r^2}{4\sigma^2}\right) \tag{3D.4}
\]

\[
\psi_{n1} (\vec{r}; D, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/4} \left( \frac{(2n)!\Gamma(D/2 + 1)}{2\Gamma(\frac{D}{2} + 1 + n)} \right)^{1/2} \left( \frac{1}{\sqrt{2\sigma}} \right) \vec{r} L_n^{D/2}(\frac{r^2}{2\sigma^2}) \exp\left(-\frac{r^2}{4\sigma^2}\right). \tag{3D.5}
\]

It is convenient to use scaled coordinates, \( \vec{Z} = \left( \frac{1}{\sqrt{2\sigma}} \right) \vec{r} \), resulting in

\[
\psi_{n0} (\vec{Z}; D) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/4} \left( \frac{\Gamma(D/2)}{2\Gamma(\frac{D}{2} + n)} (2n)! \right)^{1/2} L_n^{D/2-1}(Z^2) \exp\left(-\frac{Z^2}{2}\right) \tag{3D.6}
\]
and

\[
\overline{\psi}_{n1}(z; D) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/4} \left( \frac{\Gamma(D/2 + 1)}{\Gamma(\frac{D}{2} + 1 + n)} (2n)! \right)^{1/2} \overline{Z} L_n^{D/2}(z^2) \exp\left(-\frac{z^2}{2}\right).
\]  

(3D.7)

An important difference to note is that the argument of the Gaussian function is \( \frac{1}{2} \) that of the NC\(\mu\)-Wavelets (eq. 2.118). In the following tests of the ladder operators it will be convenient to ignore the normalization.

**Raising \( l = 0 \to 1 \), with Fixed \( n \)**

The raising operator for \( l = 0 \to 1 \) with fixed \( n \) is

\[
\alpha^+ = \frac{1}{\sqrt{2}} \left( \frac{1}{2\sigma} \overline{Z} - i\sigma \overline{k} \right).
\]  

(3D.8)

Check by application in the position representation, where the operator is

\[
\langle \overline{r} | \alpha^+ | \overline{r}' \rangle = \frac{1}{2} \left( \frac{1}{\sqrt{2}\sigma} \overline{r} - \sqrt{2}\sigma \overline{\nabla}_z \overline{r} \right)
\]  

(3D.9a)

\[
\langle \overline{z} | \alpha^+ | \overline{z}' \rangle = \frac{1}{2} \left( \overline{z} - \overline{\nabla}_z \overline{z} \right).
\]  

(3D.9b)

The effect on the operator is

\[
\alpha^+ L_n^{D/2-1}(z^2) \exp\left(-\frac{z^2}{2}\right) = \frac{1}{2} \left( \overline{z} - \overline{\nabla}_z \overline{z} \right) L_n^{D/2-1}(z^2) \exp\left(-\frac{z^2}{2}\right)
\]  

(3D.10a)

\[
= \frac{1}{2} \overline{z} L_n^{D/2-1}(z^2) \exp\left(-\frac{z^2}{2}\right) \left[ \overline{\nabla}_z \exp\left(-\frac{z^2}{2}\right) \right]
\]  

(3D.10b)

\[
= \frac{1}{2} \overline{z} L_n^{D/2-1}(z^2) \exp\left(-\frac{z^2}{2}\right) + \frac{1}{2} \left[ \overline{\nabla}_z L_n^{D/2-1}(z^2) \exp\left(-\frac{z^2}{2}\right) \right]
\]  

(3D.10c)

\[
= \frac{1}{2} \overline{Z} \left[ L_n^{D/2-1}(z^2) + L_n^{D/2-1}(z^2) \right] \exp\left(-\frac{z^2}{2}\right).
\]  

(3D.10d)
Using $L_n^{D/2} - L_{n-1}^{D/2} = L_n^{D/2-1}$ (eq. 3.35) yields

$$
\bar{\alpha}^+ L_n^{D/2-1}(Z^2) \exp\left(-\frac{Z^2}{2}\right) = -\frac{1}{2} \overrightarrow{Z} L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right). \tag{3D.11}
$$

Raising $l = 1 \to 0$, $n \to n + 1$

The raising operator for $l = 1 \to 0$ and $n \to n + 1$ is also

$$
\bar{\alpha}^+ = \frac{1}{\sqrt{2}} \left(\frac{1}{2\sigma} \overrightarrow{r} - i\sigma \overrightarrow{k}\right). \tag{3D.12}
$$

Application to the $l = 1$ state

$$
\bar{\alpha}^+ \cdot \overrightarrow{Z} L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) = \frac{1}{2} \left(\overrightarrow{Z} - \overrightarrow{\nabla}_Z\right) \cdot \overrightarrow{Z} L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) \tag{3D.13a}
$$

$$
= \frac{1}{2} Z^2 L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) - \frac{1}{2} \left[\overrightarrow{\nabla}_Z \cdot \overrightarrow{Z}\right] L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) - \frac{1}{2} \overrightarrow{Z} \cdot \overrightarrow{\nabla}_Z \left[L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right)\right] \tag{3D.13b}
$$

$$
= \frac{1}{2} Z^2 L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) - \frac{D}{2} L_n^{D/2}(Z^2) \exp\left(-\frac{Z^2}{2}\right) \tag{3D.13c}
$$

$$
+ \frac{1}{2} Z^2 \left[L_{n-1}^{D/2+1}(Z^2) + L_n^{D/2}(Z^2)\right] \exp\left(-\frac{Z^2}{2}\right) \tag{3D.13d}
$$

$$
= \frac{1}{2} \left[(2Z^2 - D) L_n^{D/2} + 2Z^2 L_{n-1}^{D/2+1}(Z^2)\right] \exp\left(-\frac{Z^2}{2}\right). \tag{3D.13d}
$$

This last expression is not one of the standard associated Laguerre recursions, but easy enough to derive. Consider the expression

$$
\overrightarrow{\nabla}_Z \cdot \left[\overrightarrow{Z} L_n^{D/2}(Z^2) \exp(-Z^2)\right] = 2(n + 1)L_n^{D/2-1}(Z^2) \exp(-Z^2), \tag{3D.14}
$$
which was obtained for the NCμ-Wavelet (eq. 3.83) by using the generator expressions. Now, evaluating by direct differentiation of the left hand side,

\[
\vec{\nabla}_Z \cdot \left[ Z L_n^{D/2}(Z^2) \exp(-Z^2) \right] = D L_n^{D/2}(Z^2) \exp(-Z^2) + \vec{Z} \cdot \left[ \nabla_Z L_n^{D/2}(Z^2) \right] \exp(-Z^2)
\]

\[
= D L_n^{D/2}(Z^2) \exp(-Z^2) - 2 \vec{Z} \cdot Z L_n^{D/2+1}(Z^2) \exp(-Z^2)
\]

\[
= 2Z \cdot \vec{Z} \cdot L_n^{D/2}(Z^2) \exp(-Z^2)
\]

results in

\[
\vec{\nabla}_Z \cdot \left[ Z L_n^{D/2}(Z^2) \exp(-Z^2) \right] = \left[ (D - 2Z^2) L_n^{D/2}(Z^2) - 2Z^2 L_{n-1}^{D/2+1}(Z^2) \right] \exp(-Z^2).
\] (3D.16)

Equating the two approaches gives a new recursion relation

\[
(D - 2Z^2) L_n^{D/2}(Z^2) - 2Z^2 L_{n-1}^{D/2+1}(Z^2) = 2(n + 1) L_{n+1}^{D/2-1}(Z^2).
\] (3D.17)

Using this results in

\[
\vec{\alpha} \cdot \vec{Z} L_n^{D/2}(Z^2) \exp(-Z^2/2) = (n + 1) L_{n+1}^{D/2-1}(Z^2) \exp(-Z^2/2).
\] (3D.18)

Lowering \( l = 1 \rightarrow 0 \), with Fixed \( n \)

The lowering operator for \( l = 1 \rightarrow 0 \) with fixed \( n \) is

\[
\vec{\alpha} = \frac{1}{\sqrt{2}} \left( \frac{1}{2\sigma} \vec{r} + i\sigma \vec{k} \right).
\] (3D.19)
which is

\[ \langle \vec{r} | \vec{\alpha} | \vec{r}' \rangle = \frac{1}{2} \left( \frac{1}{\sqrt{2\sigma}} \vec{r} + \sqrt{2\sigma} \vec{r}' \right) \]  

(3D.20a)

\[ \langle \vec{z} | \vec{\alpha} | \vec{z}' \rangle = \frac{1}{2} \left( \vec{z} + \vec{z}' \right) \]  

(3D.20b)

in the coordinate representation. Applying this lowering operator,

\[
\frac{1}{2} \left( \vec{z} + \vec{z}' \right) \cdot \vec{z} L_n^{D/2}(Z^2) \exp(-Z^2/2) \\
= \frac{1}{2} Z^2 L_n^{D/2}(Z^2) \exp(-Z^2/2) + \frac{1}{2} (D - Z^2) L_n^{D/2}(Z^2) \exp(-Z^2/2) \\
+ \frac{1}{2} Z \cdot \left[ \nabla \cdot L_n^{D/2}(Z^2) \right] \exp(-Z^2/2) \\
= \frac{1}{2} D L_n^{D/2}(Z^2) \exp(-Z^2/2) - 2 Z^2 L_{n-1}^{D/2+1}(Z^2) \exp(-Z^2/2) ,
\]  

(3D.21b)

gives

\[
\frac{1}{2} \left( \vec{z} + \vec{z}' \right) \cdot \vec{z} L_n^{D/2}(Z^2) \exp(-Z^2/2) = \frac{1}{2} \left[ D L_n^{D/2}(Z^2) - 2 Z^2 L_{n-1}^{D/2+1}(Z^2) \right] \exp(-Z^2/2) .
\]  

(3D.22)

Using eq. 3.39 results in

\[ \vec{\alpha} \cdot \vec{z} L_n^{D/2}(Z^2) \exp(-Z^2/2) = \left( n + \frac{D}{2} \right) L_n^{D/2-1}(Z^2) .
\]  

(3D.23)

**Lowering**  \( l = 0 \rightarrow 1, \ n \rightarrow n - 1 \)

The lowering operator for \( l = 0 \rightarrow 1 \) and \( n \rightarrow n - 1 \) is also

\[ \vec{\alpha} = \frac{1}{\sqrt{2}} \left( \frac{1}{2\sigma} \vec{r} + i \sigma \vec{k} \right) .
\]  

(3D.24)
Evaluating by direct application,

\[ \frac{1}{2} (Z + \nabla Z) L_n^{D/2-1}(Z^2) \exp(-\frac{Z^2}{2}) = \frac{1}{2} L_n^{D/2-1}(Z^2) \exp(-\frac{Z^2}{2}) \]

\[ + \frac{1}{2} Z \left[ -2 L_{n-1}^{D/2}(Z^2) - L_n^{D/2-1}(Z^2) \right] \exp(-\frac{Z^2}{2}) \]  \hspace{1cm} (3D.25)

results in

\[ \overline{\alpha} L_n^{D/2-1}(Z^2) \exp(-\frac{Z^2}{2}) = -L_n^{D/2}(Z^2) \] \hspace{1cm} (3D.26)
4 The Numerical Properties of the Non-Cartesian Distributed Approximating Functional

A method for analyzing a function with NCDAF is symbolized by

$$\tilde{f}(\vec{r}; M, \sigma) = \int_{\mathbb{R}^D} d\vec{r}' \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) f(\vec{r}') ,$$  \hspace{1cm} (4.1)

where \( f(\vec{r}) \) is the input function, \( \tilde{\delta}(... \) is the NCDAF parameterized by \( M \) and \( \sigma \), and \( \tilde{f}(\vec{r}; M, \sigma) \) is the filtered or "DAFed" function. An important insight can be made by taking the \( M \rightarrow \infty \) and \( \sigma \rightarrow 0 \) limits. It has been demonstrated (see chapter 2) that

$$\lim_{M \rightarrow \infty} \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) = \delta(\vec{r}' - \vec{r}) ,$$  \hspace{1cm} (4.2)

and

$$\lim_{\sigma \rightarrow 0} \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) = \delta(\vec{r}' - \vec{r}) ,$$  \hspace{1cm} (4.3)

where \( \delta(\cdots) \) is the (Dirac) delta functional [2][94]. Using the well-known property of the delta functional

$$f(\vec{r}; M, \sigma) = \int_{\mathbb{R}^D} d\vec{r}' \delta(\vec{r}' - \vec{r}) f(\vec{r}') ,$$  \hspace{1cm} (4.4)

leads to the conclusion that

$$\lim_{M \rightarrow \infty \text{ or } \sigma \rightarrow 0} \tilde{f}(\vec{r}; M, \sigma) = f(\vec{r}) .$$  \hspace{1cm} (4.5)

This means that the NCDAF approximation is exact in either one of the limits. It will be demonstrated in this chapter that for finite \( M \) and \( \sigma \) that equation 4.1 provides an accurate and robust approximation.

Before the numerical properties can be discussed, the explicit expressions for the NCDAF approximation need to be derived along with expressions for the NCDAF derivative approximation. Discussion in the chapter will be limited to the three most useful derivatives: the gradient, the Laplacian, and
the Hessian (in appendix 4A, the NCDAF Laplacian and gradient of the Laplacian approximations are
generalized to an arbitrary order). Examples of how the NCDAF can be used to approximate linear
operators are also given.

In the next two sections the numerical foundations of the continuous and discrete NCDAF will
be established. This is important for numerical applications as it shows in what sense the NCDAF
approximation is optimal. Since the goal is to approximate a function from data that are only known
at discrete grid points, a discrete NCDAF approximation is developed. In general, determining the
discrete NCDAF approximation will require a computationally costly matrix inversion. However, it will
be shown that under certain conditions the inversion can be avoided resulting a useful approximation
for the discrete NCDAF.

Next a number of numerical properties that are common to the continuous and discrete NCDAF are
discussed and demonstrated. First the special case of applying the NCDAF to polynomials is examined.
It will be shown that the NCDAF approximation, with finite $M$ (and $a$), applied to a polynomial of
appropriate degree can be made exact. Then a number of characteristics of the NCDAF error for
general smooth functions are discussed. It will be seen that in some cases the error is qualitatively
similar or even simpler than the function being approximated. Important applications such as solving
partial differential equations require robust approximation of derivatives. It will be demonstrated that
the NCDAF does indeed provide a robust approximation to derivatives that are nearly as accurate as
function approximations. The following subsection will address the nature of the convergence of the
NCDAF approximation. An important consequence is the error between sampled points of the discrete
NCDAF approximation can be made indistinguishable from the error at the sampled points. The next
topic that will be discussed is the fact that the NCDAF identity kernel is not a projection operator;
that is, the accuracy decreases with repeated approximations. Though this is a drawback, it is a trade
off which permits many of the other desirable properties. The last numerical property of the NCDAF
approximation examined is its sensitivity to discontinuities.

The final section of this chapter will be devoted to issues that arise from the discretization of the
NCDAF. It will be demonstrated that the discrete NCDAF can provide an approximation of a function between sampled points as accurate as on sampled points; that is, the NCDAF is not biased to sampled points. The importance of the NCDAF width parameter is also discussed. The major differences between the discrete and continuous NCDAF in the momentum domain is then examined. Lastly, an important limitation of the discrete NCDAF is discussed.

4.1 Expressions for NCDAF Function and Derivative Approximations

In chapter 3, the polynomial form of the NCDAF kernel was found to be

\[
\delta(\vec{r}' - \vec{r}'; M, \sigma^2) = \left(\frac{1}{2\pi\sigma^2}\right)^{D/2} \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2) \exp\left(-\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2\right),
\]

where \(Z = (1 - x)/\sqrt{2x}\), the are associated Laguerre polynomials in \(Z\). \(Z = Z^2\). \(M\) is the order of the highest such polynomial, and \(\sigma^2\) is the width parameter. It should be noted that \(\vec{r}'\) is the dependent variable and \(\vec{r}\) is a parameter (the center of the NCDAF wavepacket). The corresponding expression for the NCDAF approximation is thus

\[
\hat{f}(\vec{r}) = \left(\frac{1}{2\pi\sigma^2}\right)^{D/2} \int_{\mathbb{R}^D} d\vec{r}' \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2) \exp\left(-\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2\right)f(\vec{r}') .
\]

In the momentum domain the NCDAF approximation takes on a rather simple form. To see this take the Fourier transform of equation 4.7 noting that it is a convolution [2]. The resulting expression for the NCDAF approximation in the momentum domain is [chapter 2]

\[
\hat{F}(\vec{k}; M, \sigma) = \hat{\Delta}(\vec{k}; M, \sigma)\hat{F}(\vec{k}) ,
\]

where \(\hat{F}(\vec{k})\) is the Fourier transform of \(f(\vec{r})\) and the Fourier transform of the NCDAF is

\[
\hat{\Delta}(\vec{k}; M, \sigma) = \exp\left(-\frac{\sigma^2}{2} k^2\right) \sum_{n=0}^{M} \frac{1}{n!} \left(\frac{\sigma^2}{2} k^2\right)^n.
\]
Now consider the function $\bar{g}(\bar{r})$ which is the gradient of the function $f(\bar{r})$ symbolized by

$$\bar{g}(\bar{r}) = \nabla_{\bar{r}} f(\bar{r}).$$ \hspace{1cm} (4.10)

The DAF approximation of function $\bar{g}(\bar{r})$ is

$$NCDAF[\bar{g}(\bar{r})] = \int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}; M, \sigma) g(\{\bar{r}'\}),$$ \hspace{1cm} (4.11)

making the expression for the DAF approximation of the gradient of $f(\bar{r})$

$$NCDAF[\nabla_{\bar{r}} f(\bar{r})] = \int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}; M, \sigma) \left[\nabla_{\bar{r}} f(\bar{r}')\right].$$ \hspace{1cm} (4.12)

This expression can be integrated by parts resulting in

$$\int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}; M, \sigma) \left[\nabla_{\bar{r}} f(\bar{r}')\right] = \left[\delta(\bar{r}' - \bar{r}; M, \sigma) f(\bar{r}')\right]_{-\infty}^{\infty} - \int_{\mathbb{R}^D} d\bar{r}' \left[\nabla_{\bar{r}} \delta(\bar{r}' - \bar{r}; M, \sigma)\right] f(\bar{r}') .$$ \hspace{1cm} (4.13)

When $f(\bar{r})$ is a reasonable function, that is it does not grow faster than a polynomial in $\bar{r}$ as $|\bar{r}| \to \infty$, the surface term vanishes yielding

$$NCDAF[\nabla_{\bar{r}} f(\bar{r})] = - \int_{\mathbb{R}^D} d\bar{r}' \left[\nabla_{\bar{r}} \delta(\bar{r}' - \bar{r}; M, \sigma)\right] f(\bar{r}') .$$ \hspace{1cm} (4.14)

It is convenient to make the substitution

$$\nabla_{\bar{r}} = \nabla_{\bar{r}_R} \hspace{1cm} (4.15)$$
where $\vec{R} = \vec{r}' - \vec{r}$, giving

$$
\text{NCDAF} \left[ \nabla_{\vec{r}'} f(\vec{r}') \right] = - \int_{\mathbb{R}^D} d\vec{r}' \left[ \nabla_{\vec{R}} \delta(\vec{R}; M, \sigma) \right] f(\vec{r}') .
$$

(4.16)

Comparing equations 4.12 and 4.16 shows that the DAF approximation for the gradient of a function is equal to the gradient of the DAF approximation of the function.

The quantity

$$
- \nabla_{\vec{R}} \delta(\vec{R}; M, \sigma) = - \delta^{(1)}(\vec{r}' - \vec{r}; M, \sigma)
$$

(4.17)

is the $(M^{th}, 1^{st})$ NCDAF discussed in chapter 3. To obtain the polynomial expression for the $(M^{th}, 1^{st})$ NCDAF, start by writing the $(M^{th}, 0^{th})$ NCDAF in its polynomial form,

$$
- \nabla_{\vec{R}} \delta(\vec{R}; M, \sigma) = - \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \nabla_{\vec{R}} \left[ \sum_{n=0}^{M} Z_n^{(D/2-1)} \exp \left( - \frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) \right]
$$

(4.18a)

$$
= - \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right) \sum_{n=0}^{M} \nabla_{\vec{z}} \left[ Z_n^{(D/2-1)} \exp \left( - Z^2 \right) \right].
$$

(4.18b)

The gradient of the quantity in the [$\cdots$] brackets is given by equation 3.85 (p88), yielding

$$
- \nabla_{\vec{R}} \delta(\vec{R}; M, \sigma) = - \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{2}{\sqrt{2\sigma}} \right) \sum_{n=0}^{M} \nabla_{\vec{z}} \left[ Z_n^{(D/2)} \exp \left( - \frac{1}{2\sigma^2} \vec{R}^2 \right) \right].
$$

(4.18c)

$$
= \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{2}{\sqrt{2\sigma}} \right) \sum_{n=0}^{M} \nabla_{\vec{z}} \left[ Z_n^{(D/2)} \exp \left( - \frac{1}{2\sigma^2} \vec{R}^2 \right) \right].
$$

(4.18d)

The expression for the $(M^{th}, 1^{st})$ NCDAF kernel is thus

$$
\delta^{(1)}(\vec{r}' - \vec{r}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{2}{\sigma^2} \right)^{1/2} \sum_{n=0}^{M} \frac{1}{\sqrt{2\sigma}} \left( \vec{r}' - \vec{r} \right) L_n^{(D/2)}(Z^2) \exp \left( - \frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right)
$$

(4.19)

where it should be noted that it depends on the direction as well as the magnitude of $\vec{R}$ (i.e. it is a vector quantity). It is also important to note that the $(M^{th}, 1^{st})$ NCDAF contains a polynomial of one
higher order than the \((M^{th}, 0^{th})\) NCDAF.

Similarly, the DAF approximation of the Laplacian is equivalent to the Laplacian of the DAF applied to the input function; symbolically

\[
\text{NCDAF} \left[ \nabla^2_M f(\vec{r}) \right] = \int_{\mathbb{R}^D} d\vec{r}' \delta^{(2)}(\vec{r}' - \vec{r}; M, \sigma) f(\vec{r}') ,
\]

where the \((M^{th}, j = 2^{nd})\) NCDAF kernel is

\[
\hat{\delta}^{(2)}(\vec{r}' - \vec{r}; M, \sigma) = \nabla^2_R \hat{\delta}(\vec{R}; M, \sigma) .
\]

As before, the polynomial expression can easily be found with the results of chapter 3. Applying the Laplacian to the \((M^{th}, 0^{th})\) NCDAF kernel gives

\[
\nabla^2_R \hat{\delta}(\vec{R}; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \nabla^2_R \left[ \sum_{n=0}^M L_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) \right] .
\]

The quantity in the \{ \cdots \} bracket is given by equation 3.87 (p89), yielding

\[
\nabla^2_R \hat{\delta}(\vec{R}; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \left( \frac{1}{2\sigma^2} \right)^{n+1} \sum_{n=0}^M \sum_{n=0}^M L_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) .
\]

The expression for the \((M^{th}, 2^{nd})\) NCDAF kernel is thus

\[
\hat{\delta}^{(2)}(\vec{r}' - \vec{r}; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \left( \frac{1}{2\sigma^2} \right)^{n+1} \sum_{n=1}^{M+1} nL_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) ,
\]

where it should be noted that it is a scalar quantity. It should also be noted that the \((M^{th}, 2^{nd})\) NCDAF
kernel involves the same polynomials \((i = 0)\) as the \((M^{th}, 0^{th})\) NCDAF kernel, just shifted up by one index. The Laplacian of the NCDAF kernel therefore involves a polynomial of two degrees higher (in \(Z\)) than the original.

It is important to note that degree of the NCDAF polynomial involved increases with the order of the derivative involved. This is advantageous as the derivatives of functions, in general, increase in oscillations as derivative order is increased. Two important counter examples are polynomials and sinusoidal functions. Polynomials decrease in oscillations with increasing derivatives, and sinusoidal functions do not change in frequency upon differentiation.

Another useful derivative that can be approximated with the NCDAF is the Hessian \([106]\). As with the gradient and the Laplacian the NCDAF approximation of the Hessian acting on a function can be expressed as the Hessian acting on the NCDAF kernel as shown by

\[
\text{NCDAF} \left[ \overrightarrow{\nabla} \overrightarrow{\nabla} f(\mathbf{r}) \right] = \int_{\mathbb{R}^D} d\mathbf{r}' \left[ \overrightarrow{\nabla} \overrightarrow{\nabla} \delta(\mathbf{r}' - \mathbf{r}; M, \sigma) \right] f(\mathbf{r}) .
\]

It is possible to approximate the Hessian as the outer product of two NCDAF gradient approximations, but an elegant one step approach exists. Start be defining the \(ij^{th}\) element of the \(M^{th}\) NCDAF Hessian kernel as

\[
\delta^{(2)}_{ij}(\mathbf{r}' - \mathbf{r}; M, \sigma) = \frac{\partial}{\partial r_i} \frac{\partial}{\partial r_j} \delta(\mathbf{r}' - \mathbf{r}; M, \sigma) .
\]

It is useful to focus on the \(n^{th}\) NC\(\mu\)-Wavelet of the NCDAF kernel. Applying the first gradient (using eq. 3.85, p 88) gives

\[
\frac{\partial}{\partial Z_i} \frac{\partial}{\partial Z_j} L_n^{(D/2-1)}(Z^2) \exp(-Z^2) = \frac{\partial}{\partial Z_i} \left[ \frac{\partial}{\partial Z_j} \left\{ L_n^{(D/2-1)}(Z^2) \exp(-Z^2) \right\} \right] \quad (4.26)
\]

\[
= \frac{\partial}{\partial Z_i} \left[ -2Z_j L_n^{(D/2)}(Z^2) \exp(-Z^2) \right] . \quad (4.27)
\]

Now it is convenient to examine the two distinct types of second derivatives, the diagonal \((i = j)\) and the cross \((i \neq j)\), separately. Begin with the cross term, which evaluates (using eq. 3.42 & 3.35, p 79)
\[ 4Z_i Z_j L_n^{(D/2+1)}(Z^2) \exp(-Z^2). \] (4.28)

The diagonal terms are evaluated (using eq. 3.50, p81) as

\[ \frac{\partial}{\partial Z_i} \left[ 2Z_i I_n^{(D/2)}(Z^2) \exp(-Z^2) \right] = -2Z_i \frac{\partial}{\partial Z_i} \left[ I_n^{(D/2)}(Z^2) \exp(-Z^2) \right] - 2\delta_{ii} I_n^{(D/2)}(Z^2) \exp(-Z^2), \] (4.29)

where \( \delta_{ii} \) is the identity tensor. The diagonal terms are thus given by

\[ 4Z_i Z_i L_n^{(D/2+1)}(Z^2) \exp(-Z^2) - 2\delta_{ii} I_n^{(D/2)}(Z^2) \exp(-Z^2). \] (4.30)

Summing these new NC\(\mu\)-Wavelets gives the expression for the NCDAF Hessian kernel as

\[
\delta_{ij}^{(2)}(\overline{r}^i - \overline{r}^j; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sum_{m=0}^{M} \left( \frac{4}{2\pi\sigma} \right)^m \left( \frac{1}{2\pi\sigma} \right)^i \left( \frac{1}{2\pi\sigma} \right)^j L_n^{(D/2+1)}(Z^2) - 2\delta_{ij} I_n^{(D/2)}(Z^2) e^{-Z^2}, \]
(4.31)

where \( \delta_{ij} \) is the Kronecker delta. The recursion for the \( \alpha = D/2 + 1 \) associated Laguerre polynomials (from eq. 3.34, p 79) is

\[ (n+1) L_{n+1}^{(D/2+1)}(Z^2) = (2n - Z^2 + \frac{D}{2} + 2) L_n^{(D/2+1)}(Z^2) - (n + \frac{D}{2} + 1) L_{n-1}^{(D/2+1)}(Z^2), \] (4.32)

with the usual convention for startup terms

\[ L_{-1}^{(D/2+1)}(Z^2) = 0, \]  
\[ L_0^{(D/2+1)}(Z^2) = 1. \] (4.33)

Expressions for the NCDAF approximation for more complicated derivatives are possible. Their
derivation, however, requires knowledge of NC$\mu$-Wavelets with the appropriate rotational type. It is important to note that the NCDAF approximation of the Hessian, which is the outer product of gradients, lead to the introduction of associated Laguerre polynomials for higher order in $l$ than seen in chapter 3. Further derivations show that the Hessian can be related to the combination of NC$\mu$-Wavelets that transform a scalar and 2nd rank irreducible Cartesian tensors [103][104][107]. Higher order outer products of gradients lead to similar situations.

4.2 NCDAF Approximation of Linear Operators

In the last section it was demonstrated that the NCDAF approximation for the derivative of a function is equivalent to the convolution of the $j^{th}$ NCDAF kernel and the original function. In this sense, the $j^{th}$ NCDAF is an (integral) approximation of the $j^{th}$ gradient operator. When one realizes the identity is an operator, the $0^{th}$ NCDAF is also seen to be an operator approximation. This viewpoint can be taken advantage of to obtain the NCDAF approximation of any linear operator. In this section a few examples will be illustrated which can serve as a guide for the reader to generalize to other linear operators.

The first example is harmonic oscillator Hamiltonian [4, p481-640], symbolized by

$$H_{ho} = \frac{\hbar^2}{2m} \nabla^2 + \frac{m\omega^2}{2} r^2,$$

where $m$ is mass, $\omega$ is the spring constant and $\hbar$ is Planck’s constant divided by 2$\pi$. This operator applied to the NCDAF approximation is

$$H_{ho}\tilde{f}(\mathbf{r}'; M, \sigma) = \int_{\mathbb{R}^d} d\mathbf{r}'' \hat{H}_{ho}\delta(\mathbf{r}' - \mathbf{r}; M, \sigma) \tilde{f}(\mathbf{r}'') .$$

(4.35)
The expression for the kernel,

$$H_{ho} \delta(\vec{r}' - \vec{r}; M, \sigma) = -\frac{\hbar^2}{2m} \left[ \nabla_{\vec{r}}^2 \delta(\vec{r}' - \vec{r}; M, \sigma) \right] + \frac{m \omega^2}{2} r^2 \delta(\vec{r}' - \vec{r}; M, \sigma), \quad (4.36)$$

can be simplified by using equation 4.21 to give

$$\tilde{H}_{ho} \delta(\vec{r}' - \vec{r}; M, \sigma) = -\frac{\hbar^2}{2m} \tilde{\delta}^{(2)}(\vec{r}' - \vec{r}; M, \sigma) + \frac{m \omega^2}{2} r^2 \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma). \quad (4.37)$$

The NCDAF approximation of the harmonic oscillator Hamiltonian acting on an arbitrary state ($\psi$) is thus

$$\tilde{H}_{ho} \psi(\vec{r}) = \int_{\mathbb{R}^3} d\vec{r}' \left[ -\frac{\hbar^2}{2m} \tilde{\delta}^{(2)}(\vec{r}' - \vec{r}; M, \sigma) + \frac{m \omega^2}{2} r^2 \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) \right] \psi(\vec{r}). \quad (4.38)$$

The next example is the three-dimensional angular momentum operator [4, p641-772] which, defined in terms of its $i^{th}$ component, is

$$L_i = (r \times p)_i = -i\hbar \left( r_j \frac{\partial}{\partial r_k} - r_k \frac{\partial}{\partial r_j} \right) \epsilon_{ijk} \quad (4.39)$$

where $\times$ denotes the cross product, (bold) $\mathbf{1} = \sqrt{-1}$, $j$ and $k$ are not equal to $i$, and $\epsilon_{ijk}$ is the permutation tensor (i.e. $\epsilon_{ijk} = -\epsilon_{jik} = -\epsilon_{kji}$). Applying the angular momentum operator to NCDAF approximation,

$$L_i \tilde{f}(\vec{r}; M, \sigma) = \int_{\mathbb{R}^3} d\vec{r}' \left[ L_i \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) \right] f(\vec{r}') , \quad (4.40)$$
results in the kernel of

$$L_i \delta(\vec{r}' - \vec{r}'; M, \sigma) = -i\hbar \left( r_j \frac{\partial}{\partial r_k} \delta(\vec{r}' - \vec{r}'; M, \sigma) - r_k \frac{\partial}{\partial r_j} \delta(\vec{r}' - \vec{r}'; M, \sigma) \right) \epsilon_{ijk} \quad (4.41a)$$

$$= -i\hbar \left( r_j \delta_k^{(1)}(\vec{r}' - \vec{r}'; M, \sigma) - r_k \delta_j^{(1)}(\vec{r}' - \vec{r}'; M, \sigma) \right) \epsilon_{ijk} \quad (4.41b)$$

The NCDAF approximation of the $i^{th}$ component of the Angular Momentum operator acting on an arbitrary state is thus

$$\vec{L}_i \psi(\vec{r}) = -i\hbar \int_{\mathbb{R}^D} d\vec{r}' \left( r_j \delta_k^{(1)}(\vec{r}' - \vec{r}'; M, \sigma) - r_k \delta_j^{(1)}(\vec{r}' - \vec{r}'; M, \sigma) \right) \epsilon_{ijk} \psi(\vec{r}') \quad (4.42)$$

The last example is the quantum mechanical free evolution propagator [64] which is of the form

$$G_f = \exp \left( \psi \frac{\hbar^2}{2m} \nabla^2 \frac{\partial}{\partial r} \right) \quad (4.43)$$

where $t$ is the time parameter, and $-\frac{\hbar^2}{2m} \nabla^2 \frac{\partial}{\partial r}$ is the kinetic energy operator. The meaning of an exponentiated Laplacian can be seen when it is written in a Taylor series

$$G_f = \frac{\hbar^2}{2m} i \hbar \sum_{j=0}^{\infty} \frac{1}{j!} \nabla^2 \frac{\partial}{\partial r} \quad (4.44)$$

which clearly shows it to be a linear operator. The NCDAF approximation of the free evolution propagator is acting on an arbitrary state is thus

$$\vec{G}_f \psi(\vec{r}) = \frac{\hbar^2}{2m} i \hbar \int_{\mathbb{R}^D} d\vec{r}' \left[ \sum_{j=0}^{\infty} \frac{1}{j!} \delta^{(2j)}(\vec{r}' - \vec{r}; M, \sigma) \right] \psi(\vec{r}') \quad (4.45)$$

In this form the NCDAF free evolution propagator is not very practical because of the infinite summation. In chapter 7, an elegant and practical expression for the NCDAF Free Propagator is formulated.
4.3 Variational Derivation of NCDAF Approximation

An important concept in numerical analysis is the best approximation [28, p359-370]. It refers to the problem of choosing parameter values for an approximation method which minimizes a measurement of the error. Consider, for example, the absolute square deviation of the approximation, which is symbolized by

\[ \lambda(f, \{a\}) = \int_{\mathbb{R}^D} d\mathbf{r}' \left| f(\mathbf{r}') - \hat{f}(\mathbf{r}', \{a\}) \right|^2, \quad (4.46) \]

where \( \{a\} \) is the set of parameters and \( \hat{f} \) is the approximation of the function \( f \). To find the optimal value of the \( i \)th parameter \( (a_i) \), take the functional derivative of equation 4.46 with respect to its variation and set the result equal to zero,

\[ \frac{\delta}{\delta a_i} \lambda(f, \{a\}) = 0. \quad (4.47) \]

When \( \hat{f} \) is linear in the parameters the set of optimal values can be solved by linear algebra techniques [16, p22-98]. It is instructive to consider the example of a basis set expansion. In this method the approximation is formulated by

\[ \hat{f}(\mathbf{r}', \{a\}) = \sum_i a_i \phi_i(\mathbf{r}'), \quad (4.48) \]

where \( \phi_i(\mathbf{r}') \) are known functions and \( a_i \) are expansion coefficients. The basis functions used are usually taken to be a finite subset of a complete orthonormal set, thus making the expansion an approximation.

The functional derivative of the corresponding absolute square deviation is easily computed,

\[ \frac{\delta}{\delta a_i} \lambda(f, \{a\}) = -2 \int_{\mathbb{R}^D} d\mathbf{r}' \left( f(\mathbf{r}') - \sum_j a_j \phi_j^*(\mathbf{r}') \right) \phi_i(\mathbf{r}') = \int_{\mathbb{R}^D} d\mathbf{r}' f(\mathbf{r}') \phi_i(\mathbf{r}') - \sum_j a_j \phi_j^*(\mathbf{r}') \phi_i(\mathbf{r}'), \quad (4.49) \]

where \( * \) indicates the complex conjugate. Setting this expression equal to zero gives

\[ \int_{\mathbb{R}^D} d\mathbf{r}' f(\mathbf{r}') \phi_i(\mathbf{r}') = \int_{\mathbb{R}^D} d\mathbf{r}' \sum_j a_j \phi_j^*(\mathbf{r}') \phi_i(\mathbf{r}'). \quad (4.50) \]
Since orthonormal basis are being used, the expression yields the optimal $i^{th}$ parameter as

$$a_i = \int_{\mathbb{R}^d} d\mathbf{r}' f(\mathbf{r}') \phi_i(\mathbf{r}') .$$  \hspace{1cm} (4.51)

The reader should recognize this as the standard expression for determining the coefficients of an orthonormal basis set expansion.

Similarly the NCDAF approximation can be formulated in terms of a best approximation. Before looking at the specific case of the NCDAF, it will be instructive to first derive the expressions for the general multi-dimensional DAF. Consider the approximation of a function with basis set of the form

$$f(\mathbf{r}') = \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') ,$$  \hspace{1cm} (4.52)

where $\xi_n$ are basis functions referenced to the particular point $\mathbf{r}''$, and $a_n(\mathbf{r}'')$ are yet to be determined expansion coefficients which are likewise referenced to $\mathbf{r}''$. In this discussion it will be assumed the basis are orthogonal to their adjoint multiplied by a weight under integration. For more general cases the reader is referred to reference [22]. The weighted absolute square deviation of this approximation is

$$\lambda (\{a_n\}; \mathbf{r}'') = \int_{\mathbb{R}^d} d\mathbf{r}' w(\mathbf{r}' - \mathbf{r}'') \left| f(\mathbf{r}') - \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') \right|^2$$

$$= \int_{\mathbb{R}^d} d\mathbf{r}' w(\mathbf{r}' - \mathbf{r}'') \left( f(\mathbf{r}') - \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') \right) \times \left( f(\mathbf{r}') - \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') \right) ,$$  \hspace{1cm} (4.53a)

$$= \int_{\mathbb{R}^d} d\mathbf{r}' w(\mathbf{r}' - \mathbf{r}'') \left( f(\mathbf{r}') - \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') \right) \times \left( f(\mathbf{r}') - \sum_n a_n(\mathbf{r}'') \xi_n(\mathbf{r}' - \mathbf{r}'') \right) ,$$  \hspace{1cm} (4.53b)

where $w(\mathbf{r}' - \mathbf{r}'')$ is a weight function also referenced to point $\mathbf{r}''$, and $\times$ denotes simple multiplica-

\[\text{It should be noted that } \mathbf{r}' \text{ is the dependent variable and } \mathbf{r}'' \text{ is a parameter in this example.}\]
tion. Minimizing this with respect to the variation of each of the $a_n$ gives

$$0 = 2 \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \left( -\sum_n \left[ \frac{\delta}{\delta a_n} a_n(\vec{x}'') \right] \xi_n(\vec{x}' - \vec{x}'') \right) \times \left( f(\vec{x}') - \sum_m a_m(\vec{x}'') \xi_m(\vec{x}' - \vec{x}'') \right)$$

(4.54a)

$$0 = -2 \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \sum_n \xi_n(\vec{x}' - \vec{x}'') \left( f(\vec{x}') - \sum_m a_m(\vec{x}'') \xi_m(\vec{x}' - \vec{x}'') \right)$$

(4.54b)

$$\int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \sum_n \xi_n(\vec{x}' - \vec{x}'') f(\vec{x}') = \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \sum_n \xi_n(\vec{x}' - \vec{x}'') \left( \sum_m a_m(\vec{x}'') \xi_m(\vec{x}' - \vec{x}'') \right) .$$

(4.54c)

For one particular $n$ the expression can be written as

$$\int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \xi_n(\vec{x}' - \vec{x}'') f(\vec{x}') = \sum_m \left[ \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \xi_n(\vec{x}' - \vec{x}'') \xi_m(\vec{x}' - \vec{x}'') \right] a_m(\vec{x}'')$$

$$= \sum_m C_{nm} a_m(\vec{x}'') ,$$

(4.55a)

(4.55b)

where

$$C_{nm} = \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \xi_n(\vec{x}' - \vec{x}'') \xi_m(\vec{x}' - \vec{x}'') .$$

(4.56)

The overall equation can be put in matrix form,

$$\sum_n \int_{R^d} d\vec{x}' w(\vec{x}' - \vec{x}'') \xi_n(\vec{x}' - \vec{x}'') f(\vec{x}') = \sum_{n,m} C_{nm} a_m(\vec{x}'')$$

(4.57)

$$d = C \cdot a$$

(4.58)
where $C$ is the matrix defined above (eq. 4.56), $d$ is the vector defined by

$$d_m = \frac{1}{V} \frac{1}{(r''') - r''} C \left( r'' - r'' \right) f(\tau''), \quad (4.59)$$

and $a$ is the coefficient vector given by

$$a_m = a_m(\tau''). \quad (4.60)$$

The solution for the $a$ coefficients of this linear equation is

$$a = C^{-1} \cdot d, \quad (4.61)$$

where $C^{-1}$ is the inverse of matrix $C$. In component notation the coefficients are

$$a_m(\tau'') = \int \frac{d\tau''}{D} w(\tau'' - \tau'') \sum_n \left( C_{nm}^{-1} \right) \xi_n(\tau'' - \tau'') f(\tau''), \quad (4.62)$$

Substituting this result into equation 4.52 with $n \rightarrow m$ and $\tau'' \rightarrow \tau'$, leads to

$$\tilde{f}(\tau') = \sum_m a_m(\tau'') \xi_m(\tau' - \tau'') \quad (4.63a)$$

$$= \sum_m \left( \int \frac{d\tau''}{D} w(\tau'' - \tau'') \sum_n \left( C_{nm}^{-1} \right) \xi_n(\tau'' - \tau'') f(\tau'') \right) \xi_m(\tau' - \tau'') . \quad (4.63b)$$

It is useful to interpret this equation from a different viewpoint. When rearranged slightly,

$$\tilde{f}(\tau') = \int \frac{d\tau''}{D} \left( \sum_m w(\tau'' - \tau'') \sum_n \xi_m(\tau' - \tau'') \left( C_{nm}^{-1} \right) \xi_n(\tau'' - \tau'') \right) f(\tau'') \quad (4.64)$$
it can be seen to be in the form of

$$\tilde{f}(\vec{r}) = \int_{\mathbb{R}^D} d\vec{r}'' I(\vec{r}, \vec{r}'; \vec{r}'') f(\vec{r}'') , \quad (4.65)$$

where

$$I(\vec{r}, \vec{r}'; \vec{r}'') = w(\vec{r}' - \vec{r}'') \sum_{n,m} \xi_m(\vec{r} - \vec{r}'') (C_{nm}^{-1}) \xi_n^*(\vec{r}' - \vec{r}'') \quad (4.66)$$

is an Approximate Identity Kernel (AIK) \cite{22} parameterized by the point \(\vec{r}''\). It should be noted that this is consistent with the standard basis set expansion of the identity operator \(\text{most often called the closer relation} \ [4, \text{p122-124}], \)

$$\langle \vec{r} | \vec{r}' \rangle = \sum_n \langle \vec{r} | \phi_{n, \vec{r}''} \rangle \langle \phi_{n, \vec{r}''} | \vec{r}'' \rangle , \quad (4.67)$$

where

$$\langle \phi_{n, \vec{r}''} | \vec{r}' \rangle = w(\vec{r}' - \vec{r}'') \xi_n^*(\vec{r}' - \vec{r}'') \quad (4.68)$$

Differences in appearance are due to the inclusion of a reference point \(\vec{r}''\) and the use of biorthogonal bases \cite{108} instead of the usually orthogonal type.

It is useful to restrict attention to weight functions, \(w(\vec{r}' - \vec{r}'')\), which are a rapidly decreasing function of \(\vec{r}' - \vec{r}\). For example, \(\langle \phi_{n, \vec{r}''} | \vec{r}' \rangle\) could be harmonic oscillator wavefunctions centered about \(\vec{r}''\). When a truncated basis set is employed it should be clear points \(\vec{r}\) of the function which are closer to the reference point \(\vec{r}''\) will be approximated better than distant points.

It is possible to change the above approximation into a more uniform one. This is done by switching from using a single reference point to allowing each \(\vec{r}\) to have a different reference. The obvious choice is to use \(\vec{r}'' = \vec{r}\) thereby making each point the origin of its own basis set expansion. The resulting
is the Distributed Approximating Functional

\[ I(\vec{r}', \vec{r}'') = \sum_n b_n(0) w(\vec{r}' - \vec{r}) \xi_n^*(\vec{r}' - \vec{r}) , \]

where

\[ b_n(0) = \sum_m C_{nm}^{-1} \xi_m(0) . \]

The corresponding DAF approximation is given by

\[ \hat{f}(\vec{r}) = \int_{R^D} d\vec{r}' I(\vec{r}', \vec{r}) f(\vec{r}') \]

\[ = \int_{R^D} d\vec{r}' \left( \sum_n b_n(\vec{r}) w(\vec{r}' - \vec{r}) \xi_n^*(\vec{r}' - \vec{r}) \right) f(\vec{r}') . \]

With the groundwork prepared, the specific case of NCDAF approximation can now be discussed.

For this case, the basis functions are [see Chapter 3]

\[ \phi_n(\vec{r}' - \vec{r}) = I_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) \]

where \((\xi_n)^* = \xi_n\). The values at \(Z^2 = 0\) are given by [see section 3.1.3]

\[ \xi_n(0) = I_n^{(D/2-1)}(0) = \frac{1}{n!} \frac{\Gamma(n + D/2)}{\Gamma(D/2)} . \]
The \((n,m)^{th}\) element of the overlap matrix is thus

\[
C_{nm} = \int d\mathbf{r}' \phi_n^*(\mathbf{r}') \xi_m(\mathbf{r}') - \int d\mathbf{r}' \exp \left( -\frac{1}{2\sigma^2} (\mathbf{r}' - \mathbf{r})^2 \right) L_n^{(D/2-1)}(Z^2) L_m^{(D/2-1)}(Z^2). \tag{4.75}
\]

With a change of variables,

\[
\int d\mathbf{r}' \exp \left( -\frac{Z^2}{2} \right) L_n^{(D/2-1)}(Z^2) L_m^{(D/2-1)}(Z^2)
\]

\[
= (2\sigma^2)^{D/2} \int d\mathbf{Z} \exp \left( -\frac{Z^2}{2} \right) L_n^{(D/2-1)}(Z^2) L_m^{(D/2-1)}(Z^2), \tag{4.77}
\]

the overlap integral can be evaluated with equation 3.68 (p 85), yielding

\[
(2\sigma^2)^{D/2} \int d\mathbf{Z} L_n^{(D/2-1)}(Z^2) L_m^{(D/2-1)}(Z^2) \exp(-Z^2) = (2\sigma^2)^{D/2} \frac{1}{n!} \frac{\Gamma(n + D/2)}{\Gamma(D/2)} n^{D/2} \delta_{n,m}. \tag{4.78}
\]

The overlap matrix is thus diagonal, and the inverse is given by

\[
C_{nm}^{-1} = 1/C_{nn} = n! \frac{\Gamma(D/2)}{\Gamma(n + D/2)} \left( \frac{1}{2\sigma^2\pi} \right)^{D/2} \delta_{n,m}. \tag{4.79}
\]

With this result and the values of the polynomials the zero of its argument, the quantity

\[
b_n(0) = \sum_m C_{nm}^{-1} \xi_m(0) \tag{4.80}
\]

is determined to be

\[
b_n(0) = \frac{n! \Gamma(D/2)}{\Gamma(n + D/2)} \left( \frac{1}{2\sigma^2\pi} \right)^{D/2} \delta_{n,m} \frac{1}{n!} \frac{\Gamma(n + D/2)}{\Gamma(D/2)} \tag{4.81}
\]

\[
= \left( \frac{1}{2\sigma^2\pi} \right)^{D/2}. \tag{4.82}
\]
Inserting these results into equation 4.65 gives the NCDAF approximation as

\[ \tilde{f}(\vec{r}) = \left( \frac{1}{2\pi^D} \right)^{D/2} \int_{\mathbb{R}^D} d\vec{r}' \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2)e^{-Z^2/2}f(\vec{r}') \]. \quad (4.83)

When compared to the NCDAF approximation based on approximation of the delta functional (eq. 4.7), the two expressions are seen to be identical.

### 4.4 Discrete NCDAF Approximation

In almost all applications of interest the integral in the NCDAF approximation cannot be evaluated in a closed form. It is also common that the input function will only be known at a discrete set of points. Both these concerns necessitate a discrete version of the NCDAF. Such a generalization can be found from numerical principles analogous to those of the previous section. This will require that the integrals be replaced by weighted summations, symbolized by

\[ \int_{\mathbb{R}^D} d\vec{r}' \mapsto \sum_i \Delta_i' \]. \quad (4.84)

The quantity \( \Delta_i' \) is known as the \( i^{th} \) quadrature weight. A commonly used definition is that \( \Delta_i' \) represents the volume which is closer to the corresponding \( i^{th} \) sampled point than any other sampled point [109]. When regular grids are employed, such as will be used in the later examples, the quadrature weights are trivially calculated. For example, the quadrature weights for a 2D rectangular grid with points spaced by \( \Delta x \) and \( \Delta y \) along the x and y directions are all equal to the product \( \Delta x \Delta y \). For an arbitrary distribution of sampled points in multi-dimensions the determination of the quadrature weight can be a challenging problem [110].

The derivation of the discrete NCDAF follows the above derivation closely. It starts from the
weighted absolute square deviation of the approximation under summation instead of an integral,

\[ \lambda(\{a_n\}; \tilde{r}''') = \sum_i \Delta_i' w(\tilde{r}_i' - \tilde{r}''') \left| f(\tilde{r}_i') - \sum_n a_n(\tilde{r}''')\xi_n(\tilde{r}_i' - \tilde{r}''') \right|^2, \]  

(4.85)

where \( \tilde{r}_i' \) is the \( i^{th} \) sampled point. Since many of the steps (equations 4.53 to 4.78) are completely analogous to above\(^2\), it is economical to skip to the first point of significant difference. That point is that the expression

\[ C_{nm} = \sum_i \Delta_i' \exp \left( -\frac{1}{2\sigma^2} (\tilde{r}_i' - \tilde{r})^2 \right) L^{(D/2-1)}_n \left( \frac{1}{2\sigma^2} (\tilde{r}_i' - \tilde{r})^2 \right) L^{(D/2-1)}_m \left( \frac{1}{2\sigma^2} (\tilde{r}_i' - \tilde{r})^2 \right) \]  

(4.86)

is not equal to

\[ C_{nm} \neq (2\sigma^2)^{D/2} \frac{1}{n!} \frac{\Gamma(n + D/2)}{\Gamma(D/2)} \pi^{D/2} \delta_{n,m} = \int_{\mathbb{R}^D} d\tilde{r}' \exp \left( -\frac{1}{2\sigma^2} (\tilde{r}')^2 \right) L^{(D/2-1)}_n (\tilde{r}') L^{(D/2-1)}_m (\tilde{r}') . \]  

(4.87)

The reason is that \( L^{(D/2-1)}_n \) and \( L^{(D/2-1)}_m \) are not orthogonal under summation over a discrete set of points. It is necessary then to compute the inverse of the overlap. The discrete NCDAF approximation is thus

\[ \tilde{f}(\tilde{r}; M, \sigma) = \sum_i \Delta_i' \sum_{n=0}^M b(0) L^{(D/2-1)}_n \left( \frac{1}{2\sigma^2} (\tilde{r}_i' - \tilde{r})^2 \right) \exp \left( \frac{1}{2\sigma^2} (\tilde{r}_i' - \tilde{r})^2 \right) f(\tilde{r}_i') , \]  

(4.88)

where

\[ b(0) = \frac{C^{-1}_{nm} \frac{1}{n!} \frac{\Gamma(n + D/2)}{\Gamma(D/2)}}{\frac{1}{(2\sigma^2)^{D/2}}}, \]  

(4.89)

and \( C^{-1}_{nm} \) is defined by equation 4.86.

Under certain circumstances it is possible to avoid the costly calculation of the inverse of the overlap.

\(^2\)The reader is referred to reference [22] for details.
When the grid spacing is fine enough, equation 4.86 is approximated by

\[ C_{mn} \approx \int_{\mathbb{R}^D} d\tau^2 \exp \left( -z^2 \right) I_n^{(D/2-1)}(z^2) I_m^{(D/2-1)}(z^2) = \frac{1}{n!} \frac{\Gamma(n+D/2)}{\Gamma(D/2)} \pi^{D/2} \delta_{n,m} . \]  

(4.90)

Experience has shown that a sampling that is about 2 to 3 times finer than the Nyquist frequency is sufficient to make this approximation very accurate. The discrete NCDAF approximation then can be written as

\[ \tilde{f}(\vec{r}; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \sum_{i} \Delta_i \sum_{n=0}^{M} I_n^{(D/2-1)} \left( \frac{1}{2\sigma^2} (\vec{r}_i - \vec{r})^2 \right) \exp \left( \frac{1}{2\sigma^2} (\vec{r}_i - \vec{r})^2 \right) f(\vec{r}_i) . \]  

(4.91)

It is useful to consider a few practical issues of the discrete NCDAF approximation. Various quadrature schemes have been explored [25] but the one that has proven robust enough with acceptable computational expenditures is that of uniformly distributed grids. The most common and easily generalizable to arbitrary dimensions is rectangular sampling. More specialized examples include hexagonal [111] and triangular grids [112] in two dimensions. In the uniform grid cases, all the quadrature weights are equal (i.e. \( \Delta_i = \Delta' \)) and hence may be pulled out of the summation. Since the NCDAF kernel is a rapidly decreasing function of \( |\vec{r}' - \vec{r}| \) the summation over the sampled points can be truncated to a relatively small area. One possible rule limiting the summations is as follows. Start by defining the effective bandwidth of the NCDAF kernel as the maximum radius (in units of \( \Delta' = \Delta' \)) for which contributions with larger radius can be considered negligible. Symbolically this can be expressed as

\[ \sum_{\{ \vec{r}' \,(\Delta')^{1/D} | \vec{r}'| > W_{DAF} \}} \Delta' \sqrt{\delta(\vec{r}_i; M, \sigma)} < \varepsilon , \]  

(4.92)

where \( W_{DAF} \) is the effective bandwidth and \( \varepsilon \) a conveniently small number (e.g. \( 1 \times 10^{-32} \)). Then, for a given point \( \vec{r} \), all sampled points that fall within a bandwidth radius are to be included in the
summation; symbolically,
\[ \left\{ \frac{\sum_{i}^{r'}}{\Delta} \left( \frac{1}{\Delta^D} \right) \left| r'_i - r \right| < W_{DAF} \right\}. \]  

The expression for the discrete NCDAF with uniform sampling can then be written as
\[ f(r'; M, \sigma) = \Delta' \sum_{i}^{r'} \delta(r'_i - r'; M, \sigma)f(r'_i), \]

where
\[ \delta(r'_i - r'; M, \sigma) = \left( \frac{1}{2\pi\omega^{2}} \right)^{D/2} \sum_{i}^{M} L^{(D/2-1)} \left[ \frac{1}{2\sigma} \left( r'_i - r \right)^{2} \right] \exp \left( \frac{1}{2\sigma} \left( r'_i - r \right)^{2} \right). \]

It is important to note that this scheme gives the discrete NCDAF kernel a symmetric\(^3\) toepitz representation [44] and the approximation is in the form of a discrete convolution [16, p531-533]. All these conditions are very advantageous for computational efficiency.

### 4.5 General Numerical Properties of NCDAF Approximation

Armed with the expressions for the NCDAF function and derivative approximations and the results of the previous sections, it is now possible to discuss a number of the numerical properties of the NCDAF approximation. In a few special cases, these properties can be proven for the continuous NCDAF approximation (see for example [22], [113], and [114]); however, none rigorously carry over to the NCDAF approximation for functions that are known only as sampled points. It is thus the approach of this discussion to demonstrate through example calculations a number of properties of the approximation that are commonly observed. The conditions used will be of a relatively high density of sampled grid points thus approaching the properties of the continuous limit. More realistic computational conditions will be employed in section 4.6.

---

\(^3\) provided the parameter \( k_0 = 0 \) as is the convention of this chapter.
4.5.1 Measurement of Error

To characterize many of these properties it is convenient to define a few measurements of the error. The first is the residual function,

\[
\text{Res}(f, \vec{r}; M, \sigma) \equiv f(\vec{r}) - \hat{f}(\vec{r}; M, \sigma),
\]

which is the difference between the function and its approximation. This residual easily generalizes to the approximation of derivatives. For example, the residual of the \(j\)th gradient is

\[
\text{Res}^{(j)}(f, \vec{r}; M, \sigma) \equiv \nabla^{(j)} \frac{f(\vec{r})}{\vec{r}^j} - \hat{f}^{(j)}(\vec{r}; M, \sigma),
\]

where \(\hat{f}^{(j)}\) is the NCDAF approximation of \(j\)th gradient of the function. Another measure of error is the cost function which is defined as

\[
\text{Cost}^{(j)}(f, M, \sigma) \equiv \int_{\mathbb{R}^D} d\vec{r}^* w(\vec{r}^*) \left| \nabla^{(j)} \frac{f(\vec{r}^*)}{\vec{r}^j} - \hat{f}^{(j)}(\vec{r}^*; M, \sigma) \right|^2,
\]

or

\[
\text{Cost}^{(j)}(f, M, \sigma, \Delta') \equiv \sum_i \Delta_i w(\vec{r}_i^*) \left| \nabla^{(j)} \frac{f(\vec{r}_i^*)}{\vec{r}_i^j} - \hat{f}^{(j)}(\vec{r}_i^*; M, \sigma) \right|^2
\]

for the continuous and discrete cases respectively and \(w\) is a weight function. Unless otherwise stated the weight function is taken to be \(w = 1\) over the volume of interest and zero elsewhere. A third measure of error is the magnitude of the largest error, symbolized by

\[
\sup \left\{ \left| f^{(j)}(\vec{r}) - \hat{f}^{(j)}(\vec{r}; M, \sigma) \right|^2 : \vec{r} \in \mathbb{R}^D \right\}.
\]

4.5.2 NCDAF Approximation of Polynomials

It is instructive to examine the NCDAF approximation of polynomials by looking at a couple examples. Consider the 9th degree and 25th degree polynomials of two variables depicted in figure 4.1 and detailed
in appendix 4B. The error of the approximation is conveniently measured\(^4\) by the residual (eq. 4.96) of the form

\[
\text{Res} (f, x, y; M) = P_n (x, y) - \tilde{P}_n (x, y; M)
\]

(4.100)

where \(\tilde{P}_n\) is the NCDAF approximation of the polynomial \(P_n\). The residuals for various values of \(M\) are depicted in figures 4.2 and 4.3. It is important to note that approximations for \(P_9\) and \(P_{25}\) converge to machine precision\(^5\) at the values \(M = 4\) and 12 respectively. For the \(P_{25}\) this convergence as a function of \(M\) is rather smooth (i.e. increasing \(M\) improves the results by about an order of magnitude until convergence is reached), but for the \(P_9\) example, the error improves by several orders of magnitude when \(M\) steps from 3 to 4. These results are suggestive that polynomials are particularly well approximated by the NCDAF method. From the examples it seems that the \(M^{th}\) NCDAF approximation is sufficient to represent a polynomial of degree \(2M + 1\) accurately. Though this is not rigorously true for the discretized case, it can be proven for the continuous case.

Consider the case when the input function, \(f(\vec{r}''')\), can be written in a finite Taylor series [115]

\[
f(\vec{r}''') = \sum_{j=0}^{J} \frac{1}{(j)!} \left[ (\vec{r}''' - \vec{r}'') \cdot \nabla_{\vec{r}'''} \right]^{j} \delta (\vec{r}' - \vec{r}'') f(\vec{r}'),
\]

(4.101)

where the subscript \(\vec{r}''' = \vec{r}''\) indicates \(\vec{r}'''\) is evaluated at \(\vec{r}''\) after the derivatives have been applied. Such a function, \(f(\vec{r}''')\), is a polynomial of degree \(J\). The NCDAF approximation of such a function is given by

\[
\int_{\mathbb{R}^D} d\vec{r}''' \delta (\vec{r}''' - \vec{r}''; M, \sigma)f(\vec{r}') = \sum_{j=0}^{J} \frac{1}{(j)!} \int_{\mathbb{R}^D} d\vec{r}' \delta (\vec{r}' - \vec{r}''; M, \sigma) \left[ (\vec{r}''' - \vec{r}'') \cdot \nabla_{\vec{r}'''} \right]^{j} \delta (\vec{r}' - \vec{r}) f(\vec{r}'.
\]

(4.102)

\(^4\)since the grid is taken to be fine enough to be effectively the continuous case, the results are not particularly sensitive to the value of the parameter \(\sigma\). Therefore, it will be largely neglected from this discussion.

\(^5\)which for these cases is around \(\text{lo}10^{-14}\) to \(\text{lo}10^{-16}\), the noisy structure of the residual is an artifact of the grid spacing, the value of \(\sigma\) used, and other computational factors (such as round off errors).
Now it should be noted that $\tilde{\delta}(\cdots)$ transforms as a scalar under rotations of $\vec{r}'$, therefore, only the terms of the expansion that transform as scalars lead to nonzero contributions. In chapter 3 [section 3.1.5], it was demonstrated that the set of polynomials

$$\left\{ L_n^{(D/2-1)} (R^2) \right\}_{n = 0, 1, \cdots M} \quad (4.103)$$

where $\vec{R} = \vec{r}' - \vec{r}$, is complete for the scalar elements of a function up to degree $J \leq 2M + 1$. That is, the scalar elements of $f(\vec{r}')$ are exactly represented by the linear combination

$$\sum_{n=0}^{M>(J-1)/2} s_n L_n^{(D/2-1)} (R^2) , \quad (4.104)$$

where the expansion coefficients are given by

$$s_n = \int d\vec{R} \, e^{-R^2} L_n^{(D/2-1)} (R^2) f(\vec{r}') . \quad (4.105)$$

An alternative expansion that will be more convenient is

$$\sum_{n=0}^{M>(J-1)/2} s'_n L_n^{(D/2-1)} (Z^2) \quad (4.106)$$

where $\vec{Z} = (\vec{r}' - \vec{r}) / \sqrt{2}\sigma$ and the expansion coefficients are

$$s'_n = \int_{\mathbb{R}^D} d\vec{Z} \, e^{-Z^2} L_n^{(D/2-1)} (Z^2) f(\vec{r}')$$

$$= \left( \frac{1}{\sqrt{2\sigma}} \right)^D \int_{\mathbb{R}^D} d\vec{r}' \, e^{-Z^2} L_n^{(D/2-1)} (Z^2) f(\vec{r}') . \quad (4.107a)$$

The NCDAF representation can thus be written as

$$\tilde{f}(\vec{r}') = \sum_{n=0}^{M>(J-1)/2} s'_n \int_{\mathbb{R}^D} d\vec{r}' \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) L_n^{(D/2-1)} (Z^2) . \quad (4.108)$$
Now focus in on just the \( n^{th} \) term, which is

\[
\frac{s'_n}{2\pi\sigma^2} \int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}; M, \sigma) L_n^{(D/2-1)}(Z^2)
\]

\[
= \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} s'_n \int_{\mathbb{R}^D} d\bar{r}' \exp \left( -Z^2 \right) L_m^{(D/2-1)}(Z^2) L_n^{(D/2-1)}(Z^2)
\]

It is advantageous to change the variable of integration of \( \bar{r}' \) to \( Z \), resulting in the \((m, n)^{th}\) term being

\[
\left( \frac{1}{\pi} \right)^{D/2} s'_n \int_{\mathbb{R}^D} dZ \exp \left( -Z^2 \right) L_m^{(D/2-1)}(Z^2) L_n^{(D/2-1)}(Z^2)
\]

Now applying the orthogonality of the \( L_n^{(D/2-1)}(Z^2) \) polynomials under the weight of \( \exp(-Z^2) \) (eq. 3.68, p85) yields

\[
s'_n \left( \frac{1}{\pi} \right)^{D/2} \int_{\mathbb{R}^D} dZ \exp \left( -Z^2 \right) L_m^{(D/2-1)}(Z^2) L_n^{(D/2-1)}(Z^2) = s'_n \left( \frac{\pi}{\pi} \right)^{D/2} \frac{\Gamma(n + D/2)}{n! \frac{\Gamma(D/2)}{\delta_{m,n}}}
\]

\[
= s'_n \left( \frac{1}{n! \frac{\Gamma(D/2)}{\delta_{m,n}}} \right)
\]

This result should be compared with the effect of the exact delta functional on the polynomial set,

\[
s'_n \int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}) L_n^{(D/2-1)} \left( \frac{1}{2\sigma^2} (\bar{r}'^2 - \bar{r}^2) \right) = s'_n L_n^{(D/2-1)}(0)
\]

which using the characteristic values at zero [section 3.1.3] is

\[
s'_n \int_{\mathbb{R}^D} d\bar{r}' \delta(\bar{r}' - \bar{r}) L_n^{(D/2-1)} \left( \frac{1}{2\sigma^2} (\bar{r}'^2 - \bar{r}^2) \right) = s'_n \left( \frac{1}{n! \frac{\Gamma(n + D/2)}{\delta_{m,n}}} \right)
\]
When this result is compared with equation 4.112 it is seen that the effect of the $M^{th}$ NCDAF is the same as the exact delta functional. The consequence is that the continuous $M^{th}$ NCDAF approximation exactly represents a polynomial of degree $J \leq 2M + 1$.

### 4.5.3 General Characteristics of the NCDAF Residual of Functions

When the residuals of the example polynomials of the previous section (see figures 4.2 and 4.3) are examined closely, an interesting trend can be noted; that is, the residuals appear qualitatively like polynomials of decreasing degree as $M$ is increased to convergence. Even more interesting is the properties of the residual for a function that is not a finite power series. Consider for example the 2D sinusoidal function

$$f(x,y) = \sin \left( \frac{2\pi}{4} x + 1 \right) \cos \left( \frac{2\pi}{3} y + 1 \right) + 2,$$

which is plotted in figure 4.4. For comparison the residual for $M = 8$ NCDAF approximation is also plotted in figure 4.4. The key feature to notice is that the residual is qualitatively similar to the exact function though of significantly smaller amplitude. This is more dramatically seen in figure 4.5 where the function and a scaled (and shifted) residual are directly compared along the $x$ axis.

Though there are no rigorous proofs of these observations for the arbitrary case, it can be shown that this is what one in general should expect. Start by looking at the NCDAF approximation in the Fourier domain$^6$ [section 4.1]

$$\hat{F}(\vec{k}) = \Delta \left( \vec{k}; M, \sigma \right) F(\vec{k}). \quad (4.116)$$

The fact that $\hat{\Delta}$ is an even function of $\vec{k}$, allows it to be expanded about a reference point $\vec{k} = \vec{k}_0$ in the following manner

$$\hat{F}(\vec{k}) = \left[ \Delta(k_0^2) + (k^2 - k_0^2) \Delta^{(1)}(k_0^2) + \frac{1}{2} (k^2 - k_0^2)^2 \Delta^{(2)}(k_0^2) + \cdots \right] F(\vec{k}), \quad (4.117)$$

$^6$and it is assumed that $F(\{k\})$ exists (i.e. $f(\{r\})$ is normalizable)
where

\[
\tilde{\Delta}^{(j)}(k_0^2) = \left( \nabla_{\vec{k}}^2 \tilde{\Delta}(k^2) \right)_{k^2 = k_0^2}.
\] (4.118)

Taking the inverse Fourier transform results in

\[
\tilde{f}(\vec{r}) = \left[ \tilde{\Delta}(k_0^2) + (-\nabla_{\vec{r}}^2 - k_0^2) \tilde{\Delta}^{(1)}(k_0^2) \right] f(\vec{r}).
\] (4.119)

It is instructive to look at a typical NCDAF and its first derivative in the Fourier domain as shown in figure 4.6. One should notice that over a range of \(\vec{k}\) (the interval \((-2, 2)\) in the diagram) the NCDAF window is approximately flat making the value of the derivative near zero in that region. So for \(k_0^2\) that fall in that region, the second term in the above expansion is negligible meaning

\[
\tilde{f}(\vec{r}) \approx \tilde{\Delta}(k_0^2) f(\vec{r}), \quad (4.120)
\]

where it should be noted that \(\tilde{\Delta}(k_0^2)\) is just a number (i.e. independent of position). The residual is thus approximately

\[
R \approx \left( 1 - \tilde{\Delta}(k_0^2) \right) f(\vec{r}), \quad (4.121)
\]

that is, it is proportional to the function being approximated.

It is instructive now to examine a more complicated example. Consider the function,

\[
f(x) = e^{-x^2/20} \left( \cos \left( 2\pi x + \frac{2\pi}{5} \right) + 2 \cos \left( \frac{2\pi}{2} x + \frac{2\pi}{3} \right) \right) + 3 \cos \left( \frac{2\pi}{3} \omega x + \frac{2\pi}{2} \right) + 5 \cos \left( \frac{2\pi}{5} x + 2\pi \right) + 23,
\] (4.122)

which is plotted in figure 4.7. A scaled and shifted residual for the \(M = 0\) NCDAF approximation is also plotted in the same figure for comparison. It should be noted that though the residual does not match every feature of the function, it does reflect many aspects of the function. What appears to be missing is much of the lower frequency contributions. This conjecture is borne out when the residual
is compared with the function with the lowest frequency removed. As can be seen in figure 4.8, the residual matches the modified function better. Stepping $M$ to 1 results in a residual that matches many of the features of the function with the two lowest frequencies removed (see figure 4.9) but it is a very close match for just the highest frequency contribution (see figure 4.10). What is being observed in this example is a concept first introduced in chapter 2. That is, the frequencies (or momenta) that fall under the NCDAF momentum window where it is near unity will be represented more accurately than those falling outside. The increasing accuracy of higher frequencies is thus a result of the momentum window boarding and getting flatter as $M$ is increased.

### 4.5.4 NCDAF Approximation of Derivatives

Now the NCDAF approximation of derivatives will be demonstrated with the example function

$$f(x, y) = e^{-(x^2 + y^2)} (x^2 + y^2 - x^2 y - y) + 2,$$

(4.123)

which is plotted in figure 4.11. Plots for the gradient along $x$,

$$\frac{\partial}{\partial x} f(x, y) = e^{-(x^2 + y^2)} (-2x^3 - 2xy^2 + 2x^3 y + 2x),$$

(4.124)

gradient along $y$,

$$\frac{\partial}{\partial y} f(x, y) = e^{-(x^2 + y^2)} (-x^2 - 2x^2 y + 2x^2 y^2 + 2y + 2y^2 - 2y^3 - 1),$$

(4.125)

and the Laplacian,

$$\nabla^2 f(x, y) = e^{-(x^2 + y^2)} [4x^4 - 4x^4 y - 12x^2 y - 12x^2 y^2 + 8x^2 y^2 - 4x^2 y^3 + 6y - 12y^2 - 4y^3 + 4y^4 + 4],$$

(4.126)
are given in figures 4.12 and 4.13 respectively. Plots of the elements of the Hessian matrix,

$$
\nabla^2 f(x, y) = e^{-(x^2 + y^2)}\begin{pmatrix}
(4x^4 - 10x^2 + 4x^2y^2 + 6x^2y - 4x^3y^2 - 8xy + 2x^3) & (4x^3y + 4xy^3 - 4x^2y^2) \\
(4x^3y + 4xy^3 - 4x^2y^2) & (6x^2y - 4x^4y - 2y^2 + 2)
\end{pmatrix}
$$

are given in figure 4.14.

The NCDAF parameters for this test are chosen to fit the original function to 13 significant figures. For the example function, with the maximum amplitude of 0.8, the magnitude of the residual should be less than 1.25 \times 10^{-13}. The set of computational conditions that give this result is $\Delta_x = \Delta_y = 0.1$, $M = 11$, and $\sigma = 0.19$ as can be seen from the plot of the residual in figure 4.11.

The NCDAF approximations of the derivatives are now ready to be examined, starting with the gradient. It should be noted that this function is one of the cases where it gets more oscillatory with increasing order of derivatives (see section 4.1). With that in mind, it is encouraging to see the residuals [section 4.5.4] of the gradients along the $x$ and $y$ directions (see figure 4.12) are only about a half an order magnitude larger than that of the function approximation. The reason for such a good fit can partly be traced to the fact that $\delta^{(1)}$ incorporates a polynomial of one degree higher than $\delta^{(0)}$ [see section 4.1]. This, in effect, compensates for the added complexity of the gradient of the function.

Progressing to the Laplacian, it is seen that the magnitude of the residual (figure 4.13) is bounded by $5 \times 10^{-12}$. When the amplitude of the Laplacian of the function is taken into account (which is around 4), it is realized the fit is to about 12 significant figures. The Laplacian is thus approximated to about an order of magnitude lower accuracy than the original function. Similar is the residual for the Hessian approximation (see figure 4.15) is fit to about 12 significant figures. Experience has shown these results are typical for a wide range of test functions.

\(^7\)remember to subtract off the constant factor of 2
4.5.5 Uniform Convergence

In this section it will be shown for a broad class of functions that the NCDAF approximation converges uniformly [116]. To establish this it must be shown that 1) the magnitude of the error of the approximations is bounded by a function that is independent of position and 2) the error can be made arbitrarily small [2, p299-303]. This has been proven by Chandler & Gibson [113] and the approach taken here will be a variation on theirs.

Consider the maximum of the square deviation of the error of the NCDAF derivative approximation (eq. 4.99),

\[
\sup \left\{ \left| f^{(m)}(\vec{r}) - \tilde{f}^{(m)}(\vec{r}) \right|^2 : \vec{r} \in \mathbb{R}^D \right\} .
\] (4.128)

Restrict attention to functions \( f \) with Fourier transforms \( (\mathcal{F}F(k)) \) that have the property

\[
\int_{\mathbb{R}^D} d\vec{k} \, k^{2m} \left| \mathcal{F}F(k) \right|^2 < \infty .
\] (4.129)

In order for this to be true the square of the Fourier transformed function \( \left| \mathcal{F}F(k) \right|^2 \) must be decreasing faster than the \( m^{th} \) power of \( k^2 \) grows as \( k \to \infty \). Functions that have such a property are known as Schwartz functions \( ^8 [95][96] \). With this in mind examine the error of the derivative

\[
\nabla^{m} \int_{\mathbb{R}^D} d\vec{r}' \left( \delta(\vec{r} - \vec{r}') - \delta_n(\vec{r} - \vec{r}') \right) f(\vec{r}')
\]

\[
= \left( \frac{1}{2\pi} \right)^{D/2} \int_{\mathbb{R}^D} d\vec{k} \, e^{-i\vec{k} \cdot \vec{r}} \left( \mathcal{F}F(\vec{k}) \right)^m \left( 1 - \mathcal{F}n(\vec{k}) \right) \mathcal{F}F(\vec{k}) \delta(\vec{k} - \vec{k}') ,
\] (4.130)

where \( \delta(\vec{r} - \vec{r}') \) is the delta functional, \( \delta_n(\vec{r} - \vec{r}') \) is the \( n^{th} \) NCDAF, \( \mathcal{F}n(\vec{k}) \) is the Fourier transform

\(^8\)Schwartz functions are a little bit stronger than needed as they decrease faster than any power of \( k^2 \) not just the \( m^{th} \).
of the $n^{th}$ NCDAF. Now taking the square of each side

$$
|f^{(m)}(\vec{r}) - \tilde{f}_n^{(m)}(\vec{r})|^2 = \left( \frac{1}{2\pi} \right)^D \left| \int_{\mathbb{R}^D} d\vec{k} e^{-i\vec{k} \cdot \vec{r}} \left( i\vec{k} \right)^m \left( 1 - \tilde{\Delta}_n(\vec{k}) \right) F(\vec{k}) \delta(\vec{k} - \tilde{\vec{k}}) \right|^2 ,
$$

(4.131a)

yields

$$
\int_{\mathbb{R}^D} d\vec{k} e^{+i\vec{k} \cdot \vec{r}} \left( -i\vec{k} \right)^m \left( 1 - \tilde{\Delta}_n(\vec{k}) \right) F^*(\vec{k}) \delta(\vec{k} - \tilde{\vec{k}}') \\
\times \int_{\mathbb{R}^D} d\vec{k}' e^{-i\vec{k}' \cdot \vec{r}} \left( i\vec{k}' \right)^m \left( 1 - \tilde{\Delta}_n(\vec{k}') \right) F(\vec{k}) \delta(\vec{k}' - \tilde{\vec{k}}'')
$$

(4.131b)

$$
\int_{\mathbb{R}^D} d\vec{k} \left( \vec{k}^2 \right)^m \left( 1 - \tilde{\Delta}_n(\vec{k}) \right)^2 \left| F(\vec{k}) \right|^2 \delta(\vec{k} - \tilde{\vec{k}}')
$$

(4.131c)

$$
\int_{\mathbb{R}^D} d\vec{k} \left( 1 - \tilde{\Delta}_n(\vec{k}) \right)^2 \left| \vec{k}^m F(\vec{k}) \right|^2 \delta(\vec{k} - \tilde{\vec{k}}'')
$$

(4.131d)

The result is

$$
\sup \left\{ \left| f^{(m)}(\vec{r}) - \tilde{f}_n^{(m)}(\vec{r}) \right|^2 : \vec{r} \in \mathbb{R}^D \right\}
$$

(4.132)

$$
= \left( \frac{1}{2\pi} \right)^D \int_{\mathbb{R}^D} d\vec{k} \left( 1 - \tilde{\Delta}_n(\vec{k}) \right)^2 \left| \vec{k}^m F(\vec{k}) \right|^2 \delta(\vec{k} - \tilde{\vec{k}}'') ,
$$

which is the desired bound to the error that is independent of position (since the term containing the position exp($-i\vec{k} \cdot \vec{r}$) cancels out). Furthermore

$$
\lim_{n \to \infty} \left( 1 - \tilde{\Delta}_n(\vec{k}) \right) = 0
$$

(4.133)

for every value of $\tilde{\vec{k}}$. In chapter 2 it was shown this limit is approached smoothly, that is the sequence does not oscillate about the limit. The quantity $\tilde{\Delta}_0(\vec{k})$ starts out 1 at the origin and a plateau bounded by 1 grows outward, i.e. in the increasing $|\vec{k}|$ direction, as $n$ is incremented upwards. Since only functions that have rapidly decreasing $|\vec{k}^m F(\vec{k})|^2$ as $|\vec{k}| \to \infty$ are under considerations, the
amount of the contribution outside the plateau can be made arbitrarily small by appropriately large choices of \( n \). With the second criteria established, the uniform nature of the NCDAF approximation has been demonstrated for all functions meeting the requirement of equation 4.129.

### 4.5.6 Repeated Application of the NCDAF Approximation

A distinctive property of the NCDAF approximation is that a second application,

\[
\mathcal{R}_2 f(\mathbf{r}'; M, \sigma) = \int_{\mathbb{R}^d} d\mathbf{r''} \delta(\mathbf{r}'' - \mathbf{r}'; M, \sigma) f(\mathbf{r''}; M, \sigma),
\]

results in a new approximation that is different from the first application, i.e.

\[
\mathcal{R}_2 f(\mathbf{r}'; M, \sigma) \neq f(\mathbf{r}'; M, \sigma).
\]

Furthermore, the approximation from the second application is less accurate. Successive applications are likewise progressively less accurate.

This effect can be understood most easily by looking at the approximation in the momentum domain. The corresponding expression in the momentum domain is

\[
\hat{\mathcal{R}_2} \hat{F}(\mathbf{k}; M, \sigma) = \hat{\Delta}(\mathbf{k}; M, \sigma) \hat{\mathcal{R}_2} \hat{F}(\mathbf{k})
\]

\[
= \left[ \hat{\Delta} \hat{\Delta} \right] \hat{F}(\mathbf{k})
\]

where \( \hat{F} \) is the Fourier transform of \( f \) and \( \hat{\Delta} \) is the NCDAF kernel in the momentum domain. Since,

\[
(\hat{\Delta})^2 \neq \hat{\Delta},
\]

the NCDAF is not a projection operator. The worsening of the approximation can be seen from the
\[ \Delta - \left( \Delta \right)^2 = \Delta(1 - \Delta) . \] (4.138)

Recalling from chapter 2 that
\[ 1 \geq \Delta \geq 0 , \] (4.139)

where it is only 1 at the origin and is monotonically decreasing with increasing \[ |K| \]. The difference is thus
\[ \Delta - \left( \Delta \right)^2 > 0 , \] (4.140)

everywhere except at the origin where it is zero. The plateau for \( \left( \Delta \right)^2 \) is less wide and less flat than \( \Delta \). This fact is demonstrated in figure 4.16, where repeated multiplications of \( \Delta \) result in increasingly thinner DAF windows. These conditions lead to a less accurate approximation.

This property is a disadvantage; however, it is necessary to accept it in order to permit other desirable properties discussed below (e.g. section 4.6.1). It is possible to construct a DAF which does not degrade in accuracy upon repeat applications. Such DAFs are called interpolating DAFs [117] as they reproduce the function exactly at the grid points. The trade-off is that the approximation of a function including points off the grid will contain artifacts.

### 4.5.7 NCDAF Approximation of Discontinuities

It is instructive to examine a few examples where the behavior of the residual is significantly different than the cases looked at so far. The first is the step function
\[ f(x) = \begin{cases} 
-1 & \text{for } x < 0 \\
1 & \text{for } x \geq 0
\end{cases} , \] (4.141)

which has a major discontinuity at \( x = 0 \). Not surprisingly, approximating such a function with the DAF is problematic as can be seen in figure 4.17. Increasing \( M \) decreases the magnitude of the error.
but the approximation becomes increasingly oscillatory. The fit will only converge in the infinite $M$ limit. This is just a reflection of the well-known Gibbs phenomena [118][119]. For the second example, consider the piecewise continuous function

$$f(x) = \begin{cases} 
2 - |x| & \text{for } |x| < 1 \\
1 & \text{for } |x| \geq 1 
\end{cases}, \quad (4.142)$$

which has a discontinuous first derivatives at the points $x = 0, 1,$ and $-1$. The $M = 1$ DAF approximation of this function is plotted in figure 4.18, which is qualitatively a fairly good fit. In this case it is more insightful to examine the residual. From figure 4.19 it can be seen that there is a spike at the points $x = 0, 1,$ and $-1$, matching up with the locations of the discontinuities in the first derivative. As can be seen in figure 4.19, increasing $M$ does decrease the size of these spikes but with a corresponding increase in oscillations.

The above two examples may be academically interesting, but they are far removed from situations encountered in practical applications. Many methods for experimental measurements employ an averaging, thereby smoothing out discontinuities in the data of the function and its first derivative (and possibly higher derivatives). With this in mind, consider the function (figure 4.20)

$$f(x) = \left( x - \frac{1}{2} \right)^{5/3} \quad (4.143a)$$

$$= \left( x - \frac{1}{2} \right) \left[ \left( x - \frac{1}{2} \right)^2 \right]^{1/3}, \quad (4.143b)$$

which is continuous and has a continuous first derivative, as seen by (figure 4.21)

$$\frac{d}{dx} f(x) = \frac{5}{3} \left( x - \frac{1}{2} \right)^{2/3} \quad (4.144a)$$

$$= \frac{5}{3} \left[ \left( x - \frac{1}{2} \right)^2 \right]^{1/3}; \quad (4.144b)$$
however, the second derivative is discontinuous at the point $x = 1/2$. Like the previous example, the residual for the DAF approximation of this function (see figure 4.22) shows a spike at the point $x = 1/2$ coinciding with the discontinuity.

The reason for these results can be traced to the infinitely smooth nature of the NCDAF kernel [section 2.4]; that is, the NCDAF kernel and all its derivatives are continuous. As a consequence, the NCDAF approximation of a function is also infinitely smooth. The NCDAF is thus poor at approximating functions in the regions where there are discontinuities in the function or derivatives. This fact can be potentially turned into an advantage, as the NCDAF approximation could be used to identify the location of discontinuities in second and higher order derivatives.

4.6 Discretization Effects

4.6.1 Approximation of Functions Between Grid Points

A number of properties of the NCDAF approximation make it particularly suited for approximating functions from a discrete set of points. Consider the example calculations of derivatives with the NCDAF approximations [section 4.5.4]. Approximating the derivatives at the sampled points to a good degree of accuracy is equivalent to knowing the value of the function in the immediate neighborhood of the sampled points well. This is related to the concept that each point has its own basis set expansion [section 4.3]. The key to approximating the function at and around the sampled points is the $\sigma$ parameter of the NCDAF. One needs to choose its value small enough to make it a good approximation to the delta functional but also large enough to extend the approximation beyond the sampled points.

It is instructive now to look at an example calculation. Consider the function

$$f(x) = \frac{1}{3} e^{-\frac{1}{2}x^2} \left[ \sin \left( (5\pi) x + \frac{\pi}{2} \right) - \cos \left( (3\pi) x + \frac{\pi}{3} \right) + \cos \left( (2\pi) x + \frac{\pi}{5} \right) \right] + 2 ,$$

which has a Nyquist wavelength (see chapter 1) of about 0.2. As commented earlier [section 4.4] the NCDAF usually requires a slightly finer sampling so the value $\Delta = 0.075$ will be used. The function
with the sampled points is depicted in figure 4.23. Recall that the discrete NCDAF approximation is given by

$$\hat{f}(\mathbf{\bar{r}}; M, \sigma) = \left(\frac{1}{2\pi\sigma^2}\right)^{D/2} \sum_{(i)\Delta^{-1/2} \leq Z_{i} \leq W_{DAF}} \Delta' \sum_{n=0}^{M} L_{n}^{(D/2-1)}(2^2) \exp \left(-\frac{1}{2\sigma^2} (\mathbf{\bar{r}}'_{i} - \mathbf{\bar{r}}^2)^2\right) f(\mathbf{\bar{r}}^2)$$

(4.146)

where $\mathbf{\bar{r}}'_{i}$ are the sampled points and $\mathbf{\bar{r}}^2$ are the points of approximation. It is important to notice that this expression places no restrictions on the location of the $\mathbf{\bar{r}}'_{i}$ points. With that in mind consider the NCDAF approximation of the sampled function at the sampled points and nine intermediate points between any two of them. The residual for the set of NCDAF parameters $M = 18$ and $\sigma/\Delta = 2.10$ ($\sigma = 0.1575$) is plotted in figure 4.24. The properties to notice are: the approximation is an order of magnitude better on the grid points than off, and the approximation progressively gets worse as one moves to the center point between the sampled points. This represents a situation where the approximation is clearly biased to the sampled points. Consequence the approximation for the derivatives will be several of orders of magnitude worst than the function approximation. In order to obtain a more well-tempered approximation, one needs to sacrifice accuracy at the sampled points for overall accuracy. To ascertain how to improve the overall approximation, reexamine the results depicted in figure 4.24. The problem appears to be that the expansion about each of the sampled points does not reach far enough over the region between points. To fix this problem, try increasing the width by making the $\sigma$ parameter larger. The resulting residual for increasing $\sigma/\Delta$ to 2.25 ($\sigma = 0.16875$) is plotted in figure 4.25. The magnitude of the residual has increased but more importantly the errors on and off the grid are indistinguishable.

It is useful to put this property in perspective. Other more common approximation techniques treat the sampled points as special. For example, in polynomial methods the approximation is exact at the grid points but is oscillatory between [16, p99-102] (see figure 4.26). In contrast to these methods, the NCDAF is not restricted to be exact at the sampled points. The advantage is that the discrete NCDAF approximation can provide a well-tempered approximation [see chapter 1] that is not biased to the sampled points.
Crucial to this well-tempered approximation is the choice of the parameter $\sigma$. Since the optimal value of $\sigma$ is relative to the grid spacing, $\Delta$, it is advantageous to examine the scaled parameter $\sigma/\Delta$. It has been demonstrated elsewhere [120][121] that for given $M$ the optimal value of $\sigma/\Delta$ is largely independent of the function being approximated. Experience has shown that the DAF is optimal over a range of parameter values that make their selection a relatively easy effort.

4.6.2 Discrete NCDAF in the Momentum Domain

Discretization of the NCDAF in the position domain results in significant changes to the momentum window. Since most of the effects are independent of the number of dimensions, attention will be restricted to one dimension. The effects that depend on the number of dimensions will be discussed in a later in section 4.6.3. The discrete NCDAF in the momentum domain, $\tilde{d}$, is most conveniently expressed as a Fourier series, which is\footnote{assuming evenly spaced grid points}

\[
\tilde{d}(k; M, \sigma) = \sum_{j=-\infty}^{\infty} \exp \left(-ikx_j\right) \tilde{\delta}(x_j; M, \sigma),
\]

(4.147)

where $\tilde{\delta}$ is the discrete NCDAF kernel in the position domain (eq. 4.6). A typical example is depicted in figure 4.27. Two important features to note are 1) although the NCDAF is discrete in the position domain it is continuous in the momentum domain and 2) it is periodic with frequency of $2\pi/(\Delta x)$ where $\Delta x$ is the grid spacing. Both these features are inherent to Fourier transforms of discrete data [122]. Another difference occurs at the edges of period ($\pm \pi/(\Delta x)$). This can be seen in figure 7.28 where the discrete NCDAF is noticeably higher in amplitude than the continuous case near the edge. This effect is due to aliasing [123], where the portions of the function that fall beyond the Nyquist frequency are folded back in [16, p494-496]. It can also been seen in the same diagram that over the plateau and much of the Gaussian edges the discrete and continuous cases are effectively the same. If the essential features of the function being approximated fall under this range, then the properties of the discrete NCDAF
are essentially the same as the continuous case. This fact was used to justify the demonstration of the continuous properties in section 4.5 above. For future reference, when

$$\left| \frac{\sqrt{4M + 1}}{2(\sigma/\Delta)} \right| < \pi,$$

(4.148)

the discrete NCDAF in the momentum domain can be approximated by

$$\tilde{\Delta}_d(k) \approx \tilde{\Delta}_c(k) + \tilde{\Delta}_c\left(\frac{2\pi}{\Delta} - |k|\right),$$

(4.149)

where $\Delta$ is the grid spacing and $\tilde{\Delta}_c$ is the continuous NCDAF kernel in the momentum domain.

In section 4.4 it was mentioned that the discrete NCDAF approximation performs best with a sampling two to three times the (effective) Nyquist frequency of the function being approximated. This can now be explained in terms of the discrete NCDAF momentum window. Consider a function in the momentum domain depicted in figure 7.29a which is band-limited to $[-3, 3]$. According to the sampling theorem a grid spacing slightly larger than 1 is sufficient to exactly represent this function. The effect of a typical NCDAF momentum window with the grid spacing of $\Delta = 1$ is depicted in figure 7.29b. As can be seen this leads to significant distortion of the higher momentum values which results in a poor function approximation in the position domain. This effect can be ameliorated by using a smaller grid spacing. For example, doubling the sampling rate leads to the situation depicted in figure 7.29c. With a grid distance of $\Delta = 0.5$ the band-limited function falls entirely under the NCDAF plateau making the function approximation very good.

### 4.6.3 A Further Limitation of the Discrete NCDAF Approximation

Discretization of the NCDAF introduces a limitation on the accuracy of approximation for a given value of the $M$ parameter. In the continuous case the approximation can always be improved by either increasing $M$ or by decreasing $\sigma$. This is not true of the discrete case as $\sigma/\Delta$ values below an optimal value make the approximation worse. Consider again the approximation of function 4.145 under the...
same conditions as before except with $M = 18$ and $\sigma/\Delta = 2.00$. It should be noted that this is a smaller width than the above calculations so one would expect a better approximation on the grid points and worse off them. The results shown in figure 4.30 run counter to this assumption as even the sampled points are approximated less accurately (when compared to figures 4.24 and 4.25). It is apparent that there are limitations on the accuracy caused by concerns different from those of the section 4.6.1.

The origin of limitation is aliasing. As mentioned above, as the NCDAF momentum window spreads past the Nyquist frequency folds back in on itself. An example illustration of the effect of decreasing $\sigma$ on the discrete NCDAF momentum window is depicted in figure 4.31. It is important to notice the appearance of wings for the smallest $\sigma$ values. A close-up of the top of the plateau in figure 4.32 shows that the bumps appear at much larger values of $\sigma$. It is important to note that these wings can exceed unity and they increase in magnitude as the NCDAF approaches the limit.

It is instructive to examine this situation in cases of more than one dimension. In figure 4.33 a two dimensional discrete NCDAF momentum window with the wings is depicted. An important point that needs to be mentioned is that a square grid scheme has been employed. The resulting momentum space is square periodic. Since the NCDAF is radially symmetric there are four points nearer the edge of the period than all the rest. The effect is that the wings first appear at those points as indicated by figure 4.33.

Though these wings are usually small in magnitude they are potentially troublesome. This is especially true when a calculation requires several repeat applications of the NCDAF approximation (e.g. in dynamic calculations [34][60]-[63]). The result on the discrete NCDAF window is plotted in figure 4.34 which should be compared to the continuous case in figure 4.16. Instead of a smooth decay in accuracy the discrete approximation becomes contaminated by large distortions in the upper frequencies (momenta). The corresponding approximation is thus rendered unusable.

Experience has shown that these wings need not be totally avoided. In cases where no significant portion of the function falls near the wings there is no significant ill effect. In other cases, very good numerical results have been achieved when the excess above unity is very small (for example $1 \times 10^{-16}$).
This situation has been used as a method for optimizing the DAF parameters (see appendix 4D). The lesson to take from this is always to be careful and check for this anomaly when adjusting the DAF parameters.
Appendix 4A: NCDAF Approximation of the Arbitrary Order Laplacian and Gradient of Arbitrary Order Laplacian

In this appendix the NCDAF Laplacian approximation is generalized to an arbitrary order. The NCDAF approximation of the gradient of Arbitrary Order Laplacian is also presented. By integration by parts it can be shown that the NCDAF $j^{th}$ Laplacian approximation is

$$
NCDAF[\nabla^2_j^j f(\vec{r})] = \int_{\mathbb{R}^D} d\vec{r}' \left[ \nabla^2_j^j \delta(\vec{R}; M, \sigma) \right] f(\vec{r}) ,
$$

and the NCDAF gradient of the $j^{th}$ Laplacian approximation is

$$
NCDAF[\nabla \cdot \nabla^2_j^j f(\vec{r})] = -\int_{\mathbb{R}^D} d\vec{r}' \left[ \nabla^2_j^j \nabla^2_j^j \delta(\vec{R}; M, \sigma) \right] f(\vec{r}) .
$$

The quantities

$$
\delta^{(2j)}(\vec{r}' - \vec{r}; M, \sigma) = \nabla^2_j^j \delta(\vec{R}; M, \sigma)
$$

and

$$
\delta^{(2j+1)}(\vec{r}' - \vec{r}; M, \sigma) = -\nabla_j \nabla^2_j^j \delta(\vec{R}; M, \sigma)
$$

are the $(M^{th}, 2j^{th})$ and $(M^{th}, 2j + 1^{th})$ NCDAF kernels respectively.

To find the explicit expression for the $(M^{th}, 2j^{th})$ NCDAF kernel, start by considering the $j^{th}$ Laplacian of the NCDAF,

$$
\nabla^2_j^j \delta(\vec{R}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \nabla^2_j^j \left[ \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) \right] .
$$

$$
= \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j} \sum_{n=0}^{M} \nabla^2_j^j \left[ L_n^{(D/2-1)}(Z^2) \exp (-Z^2) \right] .
$$
The $j^{th}$ Laplacian of the quantity in the brackets is given by equation 3.93 (p90) yielding

$$\nabla_{\vec{R}}^2 \delta(\vec{R}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j} \left( -4 \right)^j \sum_{n=0}^{M} \frac{(n+j)!}{n!} L_n^{(D/2-1)}(Z^2) \exp \left( -Z^2 \right) \quad (4A.5c)$$

$$= \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j} \left( -4 \right)^j \sum_{n=j}^{M+j} \frac{n!}{(n-j)!} L_n^{(D/2-1)}(Z^2) \exp \left( -Z^2 \right). \quad (4A.5d)$$

The expression for the $(M^{th}, 2j^{th})$ NCDAF kernel is thus

$$\delta^{(2j)}(\vec{r} - \vec{r}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j} \left( -4 \right)^j \sum_{n=j}^{M+j} \frac{n!}{(n-j)!} L_n^{(D/2-1)}(Z^2) \exp \left( -Z^2 \right), \quad (4A.6)$$

where $Z = (\vec{r} - \vec{r}) / \sqrt{2\sigma}$ and it should be noted that the kernel is a scalar quantity.

Similarly, the $(M^{th}, 2j+1^{th})$ NCDAF kernel is found starting from the gradient of the $j^{th}$ Laplacian of the NCDAF,

$$\nabla_{\vec{r}} \nabla_{\vec{r}}^2 \delta(\vec{R}; M, \sigma) = -\nabla_{\vec{r}} \nabla_{\vec{R}}^2 \delta(\vec{R}; M, \sigma) \quad (4A.7a)$$

$$= - \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \nabla_{\vec{R}} \nabla_{\vec{R}}^2 \delta \left[ \sum_{n=0}^{M} L_n^{(D/2-1)}(Z^2) \exp \left( -\frac{1}{2\sigma^2} (\vec{r} - \vec{r})^2 \right) \right] \quad (4A.7b)$$

$$= - \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j+1} \sum_{n=0}^{M} \nabla_{\vec{R}} \nabla_{\vec{R}}^2 \left[ L_n^{(D/2-1)}(Z^2) \exp \left( -Z^2 \right) \right]. \quad (4A.7c)$$
By using equation 3.98 (p 92), the expression becomes

\[ \nabla_{\mathbf{r}} \nabla^{2j+1}_{\mathbf{r}} \delta(\mathbf{R}; M, \sigma) = -\left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j+1} \sum_{n=0}^{M} (-4)^j \frac{(n+j)!}{n!} \left[ \frac{\sqrt{\pi}}{Z_n^{(D/2)}} \left( Z^2 \right) \exp(-Z^2) \right] \]

(4A.7d)

\[ = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j+1} 2(-4)^j \sum_{n=j}^{M+j} \frac{n!}{(n-j)!} \left[ \frac{\sqrt{\pi}}{Z_n^{(D/2)}} \left( Z^2 \right) \exp(-Z^2) \right] . \]

(4A.7e)

The expression for the \((M^{th}, 2j + 1^{th})\) NCDAF kernel is thus

\[ \delta^{(2j+1)}(\mathbf{r}' - \mathbf{r}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \left( \frac{1}{\sqrt{2\sigma}} \right)^{2j+1} 2(-4)^j \sum_{n=j}^{M+j} \frac{n!}{(n-j)!} \left[ \frac{\sqrt{\pi}}{Z_n^{(D/2)}} \left( Z^2 \right) \exp(-Z^2) \right] , \]

(4A.8)

where it should be noted that this kernel is a vector quantity. The effect of successive gradients (and Laplacians) therefore produces a result that is more complicated, i.e. more oscillatory, than the original.
Appendix 4B: Two Dimensional Test Polynomials

In this appendix two example 2D polynomials are detailed. They are arbitrary except for having qualitatively interesting features in the region \( \{x, y\} = \{-1 \cdots -1 \cdots 1\} \). The first is a 9th degree polynomial

\[
R_b(x, y) = \frac{\left[ c_0 T_{4,0} + c_1 T_{4,1} + c_2 T_{3,2} + c_3 T_{3,3} + c_4 T_{2,4} + c_5 T_{2,5} + c_6 T_{1,6} + c_7 T_{1,7} + c_8 T_{0,8} + c_9 T_{0,9} \right]}{\sum_{i=0}^{9} |C_i|},
\]

(4B.1)

with the values

\[
\begin{align*}
    c_0 &= 9 & c_1 &= -5 & c_2 &= -2 & c_3 &= 1.5 & c_4 &= 2.5 \\
    c_5 &= -5 & c_6 &= -3 & c_7 &= 2.5 & c_8 &= -5 & c_9 &= 9
\end{align*}
\]

(4B.2)

The recursion expression for \( T_{n,i} \) is

\[
T_{n,i} = 2xyT_{(n-1),i} - T_{(n-2),i}
\]

(4B.3)

with the startup terms

\[
\begin{align*}
    T_{0,i} &= \frac{1}{2} (x^i + y^i) \\
    T_{1,i} &= xyT_{0,i}
\end{align*}
\]

(4B.4)

The example first few terms

<table>
<thead>
<tr>
<th>( n )</th>
<th>( T_{n,0} )</th>
<th>( T_{n,1} )</th>
<th>( T_{n,2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>( \frac{1}{2}(x + y) )</td>
<td>( \frac{1}{2}(x^2 + y^2) )</td>
</tr>
<tr>
<td>1</td>
<td>( xy )</td>
<td>( \frac{1}{2}(x^2y + xy^2) )</td>
<td>( \frac{1}{2}(x^3y + xy^3) )</td>
</tr>
<tr>
<td>2</td>
<td>( 2x^2y^2 - 1 )</td>
<td>( (x^2y + xy^2) - \frac{1}{2}(x + y) )</td>
<td>( (x^4y^2 + x^2y^4) - \frac{1}{2}(x^2 + y^2) )</td>
</tr>
<tr>
<td>3</td>
<td>( 4x^3y^3 + xy )</td>
<td>( 2(x^3y^2 + x^2y^3) + \frac{1}{2}(x^2y + xy^2) )</td>
<td>( 4(x^5y^2 + x^2y^5) + (x^3y + xy^3) )</td>
</tr>
</tbody>
</table>
The second example is a 25\textsuperscript{th} polynomial

\[
P_{25}(x,y) = \frac{1}{\sum_{i=0}^{25} |C_i|} [c_0 T_{13,0}^{\alpha\beta} + c_1 T_{13,1}^{\alpha\beta} + \cdots + c_{13} T_{0,13}^{\alpha\beta}]
\]

where \(T_{n,i}^{\alpha\beta}\) are a variation of the above polynomials, with the recursion

\[
T_{n,i}^{\alpha\beta} = 2xyT_{(n-1),i}^{\alpha\beta} - T_{(n-2),i}^{\alpha\beta}
\]

and startup terms

\[
T_{0,i}^{\alpha\beta} = \frac{1}{|\alpha| + |\beta|} (\alpha x^i + \beta y^i)
\]

\[
T_{1,i}^{\alpha\beta} = xyT_{0,i}^{\alpha\beta}
\]

Some example terms, with \(\gamma = |\alpha| + |\beta|\), are

<table>
<thead>
<tr>
<th>(n)</th>
<th>(T_{n,0})</th>
<th>(T_{n,1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>(\frac{1}{\gamma}(ax + \beta y))</td>
</tr>
<tr>
<td>1</td>
<td>(xy)</td>
<td>(\frac{1}{\gamma}(ax^2 y + \beta xy^2))</td>
</tr>
<tr>
<td>2</td>
<td>(2x^2 y^2 - 1)</td>
<td>(\frac{2}{\gamma}(ax^2 y + \beta xy^2) - \frac{1}{\gamma}(ax + \beta y))</td>
</tr>
<tr>
<td>3</td>
<td>(4x^3 y^3 + xy)</td>
<td>(\frac{4}{\gamma}(ax^3 y^2 + \beta x^2 y^3) + \frac{1}{\gamma}(ax^2 y + \beta xy^2))</td>
</tr>
</tbody>
</table>

\[
T_{n,2}^{\alpha\beta} = T_{n,3}^{\alpha\beta}
\]

<table>
<thead>
<tr>
<th>(n)</th>
<th>(T_{n,2}^{\alpha\beta})</th>
<th>(T_{n,3}^{\alpha\beta})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(\frac{1}{\gamma}(ax^2 + \beta y^2))</td>
<td>(\frac{1}{\gamma}(ax^3 + \beta y^3))</td>
</tr>
<tr>
<td>1</td>
<td>(\frac{1}{\gamma}(ax^2 y + \beta xy^2))</td>
<td>(\frac{1}{\gamma}(ax^4 y + \beta xy^4))</td>
</tr>
<tr>
<td>2</td>
<td>(\frac{2}{\gamma}(ax^4 y^2 + \beta x^2 y^4) - \frac{1}{\gamma}(ax^2 + \beta y^2))</td>
<td>(\frac{2}{\gamma}(ax^5 y^2 + \beta x^2 y^5) - \frac{1}{\gamma}(ax^3 + \beta y^3))</td>
</tr>
<tr>
<td>3</td>
<td>(\frac{3}{\gamma}(ax^5 y^2 + \beta x^2 y^5) + \frac{1}{\gamma}(ax^3 y + \beta xy^2))</td>
<td>(\frac{4}{\gamma}(ax^6 y^3 + \beta x^3 y^6) + \frac{1}{\gamma}(ax^4 y + \beta xy^4))</td>
</tr>
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</table>
Appendix 4C: Table of Optimal NCDAF Parameters

<table>
<thead>
<tr>
<th>$M$</th>
<th>$\sigma/\Delta$</th>
<th>$M$</th>
<th>$\sigma/\Delta$</th>
<th>$M$</th>
<th>$\sigma/\Delta$</th>
<th>$M$</th>
<th>$\sigma/\Delta$</th>
<th>$M$</th>
<th>$\sigma/\Delta$</th>
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</thead>
<tbody>
<tr>
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<td>17</td>
<td>2.19</td>
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<td>2.84</td>
<td>51</td>
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<td>18</td>
<td>2.23</td>
<td>35</td>
<td>2.88</td>
<td>52</td>
<td>3.42</td>
<td>69</td>
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<td>2.27</td>
<td>36</td>
<td>2.91</td>
<td>53</td>
<td>3.45</td>
<td>70</td>
<td>3.92</td>
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<tr>
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<td>1.52</td>
<td>20</td>
<td>2.32</td>
<td>37</td>
<td>2.95</td>
<td>54</td>
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<td>3.95</td>
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<td>2.35</td>
<td>38</td>
<td>2.98</td>
<td>55</td>
<td>3.51</td>
<td>72</td>
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<tr>
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<td>39</td>
<td>3.01</td>
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<td>40</td>
<td>3.04</td>
<td>57</td>
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<td>41</td>
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<td>58</td>
<td>3.59</td>
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<tr>
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<td>2.51</td>
<td>42</td>
<td>3.11</td>
<td>59</td>
<td>3.62</td>
<td>76</td>
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</tr>
<tr>
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<td>43</td>
<td>3.14</td>
<td>60</td>
<td>3.64</td>
<td>77</td>
<td>4.11</td>
</tr>
<tr>
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<td>1.85</td>
<td>27</td>
<td>2.58</td>
<td>44</td>
<td>3.17</td>
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<td>3.24</td>
<td>63</td>
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<td>80</td>
<td>4.17</td>
</tr>
<tr>
<td>13</td>
<td>2.00</td>
<td>30</td>
<td>2.70</td>
<td>47</td>
<td>3.27</td>
<td>64</td>
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</tr>
<tr>
<td>14</td>
<td>2.05</td>
<td>31</td>
<td>2.73</td>
<td>48</td>
<td>3.30</td>
<td>65</td>
<td>3.78</td>
<td>82</td>
<td>4.22</td>
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<td>15</td>
<td>2.10</td>
<td>32</td>
<td>2.78</td>
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<td>3.33</td>
<td>66</td>
<td>3.81</td>
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<td>16</td>
<td>2.15</td>
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<td>2.81</td>
<td>50</td>
<td>3.36</td>
<td>67</td>
<td>3.84</td>
<td>84</td>
<td>4.27</td>
</tr>
</tbody>
</table>

Where $M$ is the degree of the NCDAF polynomial (in $R^2$), $\sigma$ is the width parameter. $\Delta$ is related to the smallest period in momentum space (see section 4.6.2). For rectangular grids it is simply the largest of $\Delta_x$, $\Delta_y$, $\Delta_z$, etc. These optimal values were determined by finding the smallest value of $\sigma/\Delta$ for a given $M$ that leads to a discrete DAF in the momentum domain that does not exceed unity more than by $1 \times 10^{-15}$. These values were originally determined in [121] and have been reconfirmed for one and two dimensions. For more information please consult [120].
Figure 4.1: 9th and 25th degree polynomials of two dimensions. See appendix 4B for details.
Figure 4.2: Residuals for the 9th degree $D = 2$ polynomial.
$Res(x, y; M = 10)$

$Res(x, y; M = 11)$

$Res(x, y; M = 12)$

Figure 4.3: Residuals for the $25^{th}$ degree $D = 2$ polynomial.
Figure 4.4: Function 4.115 compared with the residual ($M = 8$ and $\sigma/\Delta = 2.0$).
Figure 4.5: Function 4.115 (solid) compared with the scaled \((x \times 10^{10} + 2)\) residual (dashed) along the \(x\) axis.
Figure 4.6: A typical NCDAF momentum window (solid) and its first derivative (dotted). Note the first derivatives is scaled by a factor of 1/2.
Figure 4.7: Function 4.122 (solid) compared with the scaled residual for $M = 0$ (dotted).
Figure 4.8: Function 4.122 with the lowest frequency contributions removed (solid) compared with the scaled residual for $M = 0$ (dotted).
Figure 5.9: Function 4.122 with the two lowest frequency contributions removed (solid) compared with the scaled residual for $M = 1$ (dotted).
Figure 4.10: Function 4.122 with only the highest frequency contribution remaining (solid) compared with the scaled residual for $M = 1$ (dotted).
Figure 4.11: Left: function 4.123. Right: the corresponding residual for $M = 11$, $\frac{\sigma}{\Delta} = 1.90$. 
Figure 4.12: Left: gradient along $x$ (top) and $y$ (bottom) directions of function 4.123 (eq. 4.124 & 4.125). Right: the corresponding residual for $M = 11$, $\sigma/\Delta = 1.90$. 
Figure 4.13: Left: Laplacian of function 4.123 (eq. 4.126). Right: the corresponding residual for $M = 11, \sigma/\Delta = 1.90$. 

\[ \nabla^2_f(x, y) \]

\[ \nabla^2_f(x, y) - f^{(R)}(x, y) \]
Figure 4.14: The elements of the Hessian matrix of function 4.123 (eq. 4.127).
Figure 4.15: Residuals of the elements of the Hessian matrix of function 4.123 (eq. 4.127) for $M = 11$, $\sigma/\Delta = 1.90$. 

\[ \frac{\partial^2}{\partial x \partial y} f(x, y) - f^{(2)}_{xy}(x, y) \]

\[ \frac{\partial^2}{\partial x^2} f(x, y) - f^{(2)}_{xx}(x, y) \]

\[ \frac{\partial^2}{\partial y^2} f(x, y) - f^{(2)}_{yy}(x, y) \]
Figure 4.16: Effect of repeated multiplications of the NCDAF window in momentum domain. The outmost is the original window, and after $1, 10, 100, 1\times10^4,$ and $1\times10^6$ repeated multiplications for each successively inner plot.
Figure 4.17: Function 4.141 (solid) and the DAF approximations for $M = 0$ (dashed), 4 (dotted), and 128 (dot-dashed).
Figure 4.18: Top: function 4.142. Bottom: detail of function (solid) and DAF approximation for $M = 1$ (dashed).
Figure 4.19: Residuals for function 4.142.
Figure 4.20: Top: function (eq. 4.143) with discontinuous 2nd derivative at point $x = 0.5$. Bottom: detail of function (solid) compared with the DAF approximation for $M = 0$ (dashed).
Figure 4.21: First derivative of function 4.143 which is continuous but problematic at the point $x = 0.5$. 


Figure 4.22: Residual ($M = 0$) of function 4.143 clearly indicating a problematic point $x = 0.5$. 

Figure 4.23: Function 4.145 showing sampled points (circled).
Figure 4.24: Residual of function 4.145 on (circled) and off sampled points for $M = 18$ and $\sigma/\Delta = 2.10$
Figure 4.25: Residual of function 4.145 on (circled) and off sampled points for $M = 18$ and $\sigma/\Delta = 2.25$. 
Figure 4.26: Example of a typical interpolation method which treat the sampled points as special. Note the error is zero at the grid points and reaches maximum values about half-way between the grid points.
Figure 4.27: Discrete NCDAF window in the momentum domain for $M = 8$ and $\sigma/\Delta = 1.75$. Horizontal axis in units of $1/\Delta$ where $\Delta$ is the grid spacing.
Figure 4.28: Comparison of continuous (solid) and discrete (dotted) DAF Kernels in the momentum domain. The parameters used are $M = 8$ and $\sigma = 1.75$ for both cases.
Figure 4.29: Effect of the discrete NCDAF momentum window \((M = 8 \text{ and } \sigma/\Delta = 1.75)\) on a band-limited function: (a) function in momentum domain with is band-limited to \([-3, 3]\), (b) multiplied by NCDAF momentum window with grid spacing of \(\Delta = 1\), and (c) multiplied by NCDAF momentum window with grid spacing of \(\Delta = 0.5\).
Figure 4.30: Residual of function 4.145 on (circled) and off sampled points for $M = 18$ and $\sigma/\Delta = 2.00$. 
Figure 4.31: Illustration of the behavior of discrete NCDAF as its width parameter ($\sigma$) is decreased:

$\sigma = 4.00$ (solid), $\sigma = 3.50$ (dashed), $\sigma = 3.00$ (dotted), $\sigma = 2.90$ (dot-dashed), $\sigma = 2.88$ (dot-dot-dashed), $\sigma = 2.87$ (solid). In all cases $M = 40$. 
Figure 4.32: Detail of discrete NCDAF window in momentum domain with $M = 40$ and $\sigma/\Delta = 2.90$. 
Figure 4.33: Detail of discrete NCDAF window in momentum domain for two dimensions with $M = 18$ and $\sigma/\Delta = 2.00$. 
Figure 4.34: Effect of repeated multiplications of the discrete NCDAF window in momentum domain with poor choice of parameters $M = 18$ and $\sigma/\Delta = 2.00$. The windows are after 10 (solid), 1000 (dashed), and $1 \times 10^4$ (dotted) repeated multiplications. Horizontal axis in units of $1/\Delta$ where $\Delta$ is the grid spacing.
5 Comparison of Non-Cartesian and Cartesian Product Distributed Approximating Functionals

The most common approach for generalizing approximation and analysis methods to multi-dimensions is to employ Cartesian products of one-dimensional functions. The main reason for this is that the generalization is almost trivial due to the translational symmetry present in each variable. Adaptations of one-dimensional codes are then very straightforward. Many properties of the one-dimensional functions can easily be shown to hold in a Cartesian product.

Using direct products of one-dimensional functions, however, has a major drawback. They introduce a preferred orientation. For data that possess a product structure that coincides with this bias it is an advantage. The problem is that the vast majority of natural phenomena do not have an underlying product structure. The manifestations of this unnatural bias are 1) the error will be a function of orientation of the product axis relative to the data, and 2) an artificial rectangular structure is introduced into the approximation. This can lead to artifacts which have been noted to be problematic in a number of challenging areas such as data compression and image analysis [23].

In this chapter the NCDAF will be compared with the Cartesian-Product DAF (CPDAF) [60]. First, details of the CPDAF are discussed and qualitative differences with the NCDAF are examined. In the second section, the interrelationships between the NCDAF and CPDAF are detailed. The next section discusses some general conditions under which the two methods can be considered equivalent. The fourth section compares computational efficiency of the two approaches. In the fifth section a distinct difference seen in the approximation of polynomials is explored. In the sixth section it is demonstrated that, unlike the NCDAF, the CPDAF approximation is dependent on the choice of axis. The last section demonstrates the artificial rectangular structure that product methods can induce in approximations.

Attention will be restricted to examples in two dimensions, but the results easily generalize to higher dimensions. To simplify the comparison of the two approaches, only cases where $M_1 = M_2 = M_{CP}$ will be considered. Similarly, cases will be restricted to where the CPDAF is characterized by a single
width parameter, i.e. \( \sigma_1 = \sigma_2 = \sigma_{CP} \).

### 5.1 Cartesian Product DAF

The Cartesian Product DAF is simply the product of one-dimensional DAFs given by

\[
\delta_{CP}(\vec{r}' - \vec{r}; \{M\}, \{\sigma\}) = \delta(x'_1 - x_1; M_1, \sigma_1) \delta(x'_2 - x_2; M_2, \sigma_2) \cdots \delta(x'_D - x_D; M_D, \sigma_D),
\]

with

\[
\delta(x'_i - x_i; M_i, \sigma_i) = \left( \frac{1}{2\pi \sigma_i^2} \right)^{1/2} \sum_{n_i=0}^{M_i} \left( \frac{-1}{4} \right)^{n_i} \frac{1}{(n_i)!} \left( \sqrt{2\sigma_i} \frac{\partial}{\partial x_i} \right)^{2n} \exp \left( -\frac{1}{2\sigma_i^2} (x'_i - x_i)^2 \right),
\]

where \( D \) is the number of dimensions, \( M_i \) and \( \sigma_i \) are the DAF parameters for the \( i^{th} \) component, and \( L_{n_i}^{(-1/2)} \) are associated Laguerre with a squared argument [see chapter 3]. In the momentum domain the CPDAF is of the form

\[
\tilde{\delta}_{CP}(\vec{k}; \{M\}, \{\sigma\}) = \tilde{\Delta}(k_1; M_1, \sigma_1) \tilde{\Delta}(k_2; M_2, \sigma_2) \cdots \tilde{\Delta}(k_D; M_D, \sigma_D),
\]

where

\[
\tilde{\Delta}(k_i; M_i, \sigma_i) = \exp \left( -\frac{\sigma_i k_i^2}{2} \right) \sum_{n_i=0}^{M_i} \frac{1}{(n_i)!} \left( \frac{\sigma_i k_i^2}{2} \right)^{n_i}.
\]

It should be noted that the shape of the momentum window along any axis is identical to the one-dimensional window.

A typical CPDAF kernel for two dimensions is depicted in figure 5.1. For comparison a typical NCDAF kernel is also plotted in the same figure. The most remarkable difference is the rectangular structure of the CPDAF compared to the spherical structure of the NCDAF. This is also seen in the
kernels in the momentum domain as can be seen in figure 5.2. These qualitative differences are a reflection of the CPDAF's bias to a choice of axis.

As the set of $M$ values approaches $\infty$ or the set of $\sigma$ values approach 0, the CPDAF becomes

$$\lim_{\{M\} \to \infty \text{ or } \{\sigma\} \to 0} \tilde{\delta}_{CP}(\vec{r}' - \vec{r}; \{M\}, \{\sigma\}) = \delta(x'_1 - x_1)\delta(x'_2 - x_2) \cdots \delta(x'_D - x_D) \quad (5.6)$$

where $\delta(x_i - x_i)$ is a one-dimensional (Dirac) delta functional.

An important difference of the CPDAF is that its DAF parameters, $M_i$ and $\sigma_i$, can vary for each dimension. This is advantageous for approximating functions which are more oscillatory along particular directions that intersect at right angles. It should be noted that it is possible to construct a NCDAF approximation that employs different levels of approximation along different directions [100]. This is done by introducing anisotropic NCDAF width parameters and scaled coordinates.

5.2 Interrelationship Between CP and NCDAFs

It is instructive to examine the interrelationships of the Cartesian Product and Non-Cartesian DAF approaches. An important situation that the relationships show is when one type of DAF is completely incorporated in the other. In terms of the corresponding momentum windows, this means that one approach completely bounds the other. Furthermore, the bounding approach is wider in momentum with a plateau that is closer to the ideal window. The consequence of this [see section 2.4] is that the bounding approach will be a better approximation in terms of the smaller cost function [section 4.5.1, eq. 4.98].

In two dimensions the $M^{th}$ CPDAF kernel in the momentum domain can be written as (see appendix 5A)

$$\tilde{\Delta}_{CP}(k_x, k_y; M, \sigma) = \tilde{\Delta}_{NC}(k_x, k_y; M, \sigma)$$

$$+ \sum_{n=1}^{M} \sum_{m=M-n+1}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} \left( k_x^2 + k_y^2 \right) \right), \quad (5.7)$$
where $\Delta_{NC}$ is the $M^{th}$ NCDAF kernel and it is important to note that $\sigma_{CP} = \sigma_{NC} = \sigma$. This means that the $M^{th}$ NCDAF kernel is completely contained within the $M^{th}$ CPDAF. This is demonstrated in figure 5.4 where the $4^{th}$ CPDAF is shown to completely bound the $4^{th}$ NCDAF momentum window.

It is useful to show how the restriction $\sigma_{CP} = \sigma_{NC}$ can be relaxed. First it should be remembered that the shape of the $M^{th}$ NCDAF momentum window along the diameter is the same as the $M^{th}$ one-dimensional DAF [section 2.4]. Likewise, the $M^{th}$ CPDAF along the $x$-axis (or $y$-axis) is the same shape the $M^{th}$ one-dimensional DAF. It is thus sufficient to consider the effect of changing $\sigma$ in just one dimension. In section 2.4, it was shown that, for a fixed $M$, a smaller value of $\sigma$ leads to a momentum window that completely bounds one with a larger $\sigma$ value. From this it can be concluded that the $M^{th}$ CPDAF kernel bounds the $M^{th}$ NCDAF kernel provided that $\sigma_{CP} \leq \sigma_{NC}$.

In two dimensions the $2M^{th}$ NCDAF kernel in the momentum domain can be written as (see appendix 5A)

$$\tilde{\Delta}_{NC}(k_x, k_y; 2M, \sigma) = \Delta_{CP}(k_x, k_y; M, \sigma)$$

$$+ \sum_{n=0}^{M-1} \sum_{m=M+1}^{2M-n} \frac{1}{n!} \left( \frac{\sigma_x^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma_y^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right)$$

$$+ \sum_{m=0}^{M-1} \sum_{n=M+1}^{2M-m} \frac{1}{n!} \left( \frac{\sigma_x^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma_y^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right),$$

where $\sigma_{CP}$ is restricted to be equal to $\sigma_{NC}$. This means that the $M^{th}$ CPDAF is completely contained within the $2M^{th}$ NCDAF kernel. This is demonstrated in figure 5.3 where the $6^{th}$ NCDAF completely bounds the $3^{rd}$ CPDAF momentum window. As before the restriction on the widths can be relaxed. In this case, $\sigma_{CP} \geq \sigma_{NC}$ is required for the $2M^{th}$ NCDAF kernel to completely bound the $M^{th}$ CPDAF kernel.

It is useful in certain instances to employ an alternative viewpoint for the relationship of the CP and NCDAF approaches. An important example is the approximation of polynomials which will be discussed below. Since polynomials are not analyzable by Fourier methods, comparing DAF kernels in
the momentum domain is not insightful. In these cases the characteristics of the NCDAF and CPDAF are best examined in the position domain.

A position domain relationship can be formulated by using polynomial term diagrams for the two types of DAFs. Now, consider the example term diagrams

\[
\begin{array}{c|c}
\text{4th CPDAF} & \text{4th NCDAF} \\
\hline
6 & 6 \\
5 & 5 \\
4 & 4 \\
3 & 3 \\
2 & 2 \\
1 & 1 \\
0 (a) & 0 (a) \\
1 & 1 \\
2 & 2 \\
3 & 3 \\
4 & 4 \\
5 & 5 \\
6 & 6 \\
\end{array}
\]

where a dot (●) indicates that a term proportional to \( x_1^{a} x_2^{b} \) is included in the DAF kernel. An important difference between the two methods is apparent from these diagram. Although the NCDAF includes all terms up to a given total degree \( (a_{\text{max}} + b_{\text{max}} = M) \), the CPDAF includes terms generated from the product of \( x_1^{a} \) and \( x_2^{b} \) where \( \{a : 0 \cdots M\} \) and \( \{b : 0 \cdots M\} \). The term diagrams are useful for showing the similarities of the two methods. Consider the combined diagram

\[
\begin{array}{c|c}
\text{4th CPDAF} & \text{4th NCDAF} \\
\hline
6 & 6 \\
5 & 5 \\
4 & 4 \\
3 & 3 \\
2 & 2 \\
1 & 1 \\
0 (a) & 0 (a) \\
1 & 1 \\
2 & 2 \\
3 & 3 \\
4 & 4 \\
5 & 5 \\
6 & 6 \\
\end{array}
\]

of the 4th CPDAF and 4th NCDAF where ● indicated common terms and ○ indicated terms unique.

\(^1\text{recall that the DAF kernels only include terms that transform as scalars and hence only even powers of }x_1 \text{ and } x_2\)
to the CPDAF. It is important to note that although some terms are shared, the coefficients for these terms are different for each method. Since the CPDAF depicted in this diagram contains all the terms of the NCDAF depicted, the CPDAF will lead to a better approximation than the NCDAF (provided $\sigma_{NC} \geq \sigma_{CP}$). Now consider the combined term diagram of the $3^{rd}$ CPDAF and $6^{th}$ NCDAF where $\bullet$ indicates common terms and $\bigcirc$ indicates terms unique to the NCDAF. In this case the NCDAF approximation will be the more accurate of the two approaches in terms of the cost functions (provided $\sigma_{NC} \leq \sigma_{CP}$).

5.3 Equivalence of CPDAF and NCDAF Approximations

In the last section, the conditions which make either the CPDAF or NCDAF the more accurate approach were found. The natural question that arises is under what conditions are the CPDAF and NCDAF equivalent. In general the answer will depend on the function being approximated, in the absence of that knowledge one can find some rough equivalences. The simplest way is to consider any pair of NCDAF and CPDAF where neither bounds the other to be equivalent. For example, the $4^{th}$ NCDAF and the $3^{rd}$ CPDAF fall under this category (see figure 5.5). In this section two, more sophisticated, equivalence viewpoints are discussed. The first is based on the properties of the DAF in the momentum domain and second on properties of the DAFs in the position domain.
5.3.1 Momentum Plateau Viewpoint

Consider the NCDAF and CPDAF kernels in the momentum domain (e.g. figure 5.2). The key feature with important consequences for the accuracy of the approximation is the area of the momentum window which is near unity. An estimate\(^2\) of this area in two dimensions for the NC approach is given by

\[
A_{NC} = \pi k_r^2, \quad (5.12)
\]

and for the CP approach by

\[
A_{CP} = 4k_r^2, \quad (5.13)
\]

where

\[
k_r^2 = \frac{(4M + 3) - \sqrt{16M + 9}}{2\sigma^2}. \quad (5.14)
\]

This quantity \((k_r^2)\) corresponds to the momentum value along the axis where a rapid transition in \(|\vec{k}|\) begins which indicates the end of the plateau (see figure 2.11). For details of \(k_r^2\)'s derivation the reader is referred to appendix 2C.

As discussed in chapters 2 and 4, the better the approximation the larger the area of the momentum window which is near unity. A reasonable choice for equivalence between the CPDAF and NCDAF approaches is when the area of their respective plateaus are about the same. When \(M_{NC} = M_{CP}\) this occurs (by using eq. 5.14, 5.12, and 5.13) when

\[
4\sigma_{NC}^2 = \pi\sigma_{CP}^2. \quad (5.15)
\]

For cases where \(\sigma_{NC} = \sigma_{CP}\), the equivalence only occurs at \(M_{NC} = M_{CP} = 0\). Equivalence in other cases needs to be determined on a case by case basis. For example the area of the plateau for the 4th

\(^2\)A more accurate estimate is based on the points of maximum curvature. This expression is not as convenient as points of rapid transition. See appendix 2C for details.
NCDAF and the 3\textsuperscript{rd} CPDAF is the same when

$$\sigma_{NC}^2 \approx 1.12 \sigma_{CP}^2.$$  \hfill (5.16)

It should be mentioned that this viewpoint is not without its limitations. It is possible for a momentum window that bounds at the top of the plateau to be exceeded at the foot of the cliff. This is illustrated in figure 5.6. This is especially likely when the $M$ values of the two approaches are significantly different and a smaller $\sigma$ is associated with the larger $M$. In such cases, it is best to check the overall shape of the two DAF kernels in the momentum domain.

5.3.2 Polynomial Term Diagram Viewpoint

An alternative viewpoint for the equivalence of the two approaches is based on their polynomial term diagrams. In general the more terms that are included in an approach the better the approximation should be (see section 5.5 for an example). A CPDAF kernel and NCDAF kernel with roughly the same number of terms will be considered equivalent. Consider the example term diagrams

It should be noticed that the 3\textsuperscript{rd} CPDAF has 16 terms and the 4\textsuperscript{th} NCDAF has 15 terms making them roughly equivalent. Experience has confirmed that CPDAF and NCDAF which are equivalent under this viewpoint deliver comparable levels of accuracies.
5.4 Computational Efficiency

Efficiency of a numerical method can be characterized by two distinct concerns. They are memory usage and speed of calculation. Obviously the smaller the storage requirement and the faster the calculation the more efficient the method. In general a comparison of efficiency can be rather complicated, but since the computational differences between the NCDAF and CPDAF approximation methods are small many of the details can be ignored. Memory use can simply be measured in the number of unique elements of the DAF matrix. Speed is also easily quantified as the number of DAF polynomial recursions. In the discussion below it will be assumed that function being approximated is two dimensional and not separable into two one-dimensional functions.

It is instructive first to review a few basic DAF concepts. The discretized expressions for the NC approach is [section 4.4]

\[
\tilde{f}_{NC}(x, y; M, \sigma) = \left( \sum_{\{i \mid |\bar{r}_i - \bar{r}| \leq R_{DAF} \}} \Delta_i \tilde{\delta}_{NC}(\bar{r}_i - \bar{r}; M, \sigma) \right) f(x_i^*, y_i^*),
\]

where \( R_{DAF} \) is a cut-off radius, \( \Delta_i \) is the quadrature weight of the \( i^{th} \) sampled point (\( \bar{r}_i \) or \( x_i^*, y_i^* \)), and \( \tilde{\delta}_{NC} \) is the NCDAF kernel. The discretized expressions for the CP approach is

\[
\tilde{f}_{CP}(x, y; M, \sigma) = \left( \sum_{\{j \mid |x_j - x| \leq R_{DAF} \}} (\Delta x_j^*) \tilde{\delta}(x_j^* - x; M, \sigma) \right) f(x_j^*, y_k),
\]

\[
\times \left( \sum_{\{k \mid |y_k - y| \leq R_{DAF} \}} (\Delta y_k^*) \tilde{\delta}(y_k^* - y; M, \sigma) \right) f(x_j^*, y_k),
\]

where \( \Delta x_j^* \) and \( \Delta y_k^* \) are the quadrature weights along the \( x \) and \( y \) directions respectively and \( \tilde{\delta} \) are the one-dimensional DAF kernels. It should be noted that the summations as written above do not cover the same exact number of points. This can be corrected (without introducing a significant error) by
using a refined summation rule for the CP approach of

\[ \left\{ j,k \mid \sqrt{(x'_j - x)^2 + (y'_k - y)^2} \leq R_{DAF} \right\} . \] (5.20)

The corresponding DAF matrices of the two methods thus have the same number of elements which are (effectively) nonzero. The important features to note are 1) NC is a function of one distance while the CP is a function of two and 2) NCDAF involves one \( M_{NC} \) degree polynomial (in \( \frac{1}{2\pi^2} R^2 \)) and the CPDAF involves two \( M_{CP} \) degree polynomials (in \( \frac{1}{2\pi^2} x^2 \) and \( \frac{1}{2\pi^2} y^2 \)). It is common practice to employ uniform grids meaning that the quadrature weights are independent of position (i.e. \( \Delta'_j = \Delta' \), \( \Delta x'_j = \Delta x' \), and \( \Delta y'_k = \Delta y' \)). In such cases it is convenient to characterize the bandwidth of the DAF by

\[
W_{DAF} = \Phi(R_{DAF}/\Delta')
\]

\[
W_{x,DAF} = \Phi(R_{DAF}/\Delta'_x),
\]

\[
W_{y,DAF} = \Phi(R_{DAF}/\Delta'_y)
\]

where \( \Phi(\cdots) \) is a function that takes on the value of its argument rounded up to the next integer. The bandwidth of the NCDAF kernel is thus

\[ 2W_{DAF} + 1 , \] (5.22)

and for the CPDAF is

\[ 2W_{x,DAF} + 1 \text{ and } 2W_{y,DAF} + 1 . \] (5.23)

It will be convenient to the discussion to make the assumption that the bandwidth of the CP and NP approaches is the same for approximations of equivalent accuracy.

A major factor that effects memory efficiency is symmetry of the grid. Consider a 2 dimensional grid laid out in a regular square mesh. In this case the two CPDAF kernels are identical (since \( \Delta'_x = \Delta'_y \)) meaning there are only \( W_{DAF} + 1 \) unique elements to be stored. The number of unique elements for the
NCDAF kernel can be rather complicated to express, but a good upper estimate is \( \frac{1}{2} \left( W_{D_A} + 1 \right)^2 + \frac{1}{2} \left( W_{D_A} + 1 \right) \). The CP approach is clearly more efficient with respect to memory for the square mesh. The situation is similar for rectangular meshes as the number of stored elements for both approaches increase by about a factor of 2. For cases where one wishes to approximate a function at arbitrary positions, there are no unique elements in either approach. In such cases the storage efficiency of the CPDAF over the NCDAF vanishes.

When approximations are made on regular grid meshes the bottleneck (i.e. point of most significant slowdown) of the calculation is the summations in equations 5.18 and 5.19. Since the summations are over the same exact number of points the speed efficiency of the CPDAF and NCDAF are essentially the same. When the approximations are required are arbitrary points, the bottleneck becomes the polynomial evaluations. For the NCDAF approach this is \( M_{NC} - 1 \) (for \( M_{NC} > 1 \), the \(-1\) is due to the startup terms which are evaluated directly\(^3\)) and for the CPDAF approach this is \( 2M_{CP} - 2 \) (for \( M_{CP} > 1 \)). It is instructive to consider an example. In the last section it was determined that the \( M = 4 \) NCDAF and the \( M = 3 \) CPDAF are roughly equivalent in terms of accuracy. Using the expressions it is seen that

\[
\begin{array}{ccc}
M = 4 \text{ NCDAF} & 3 \\
M = 3 \text{ CPDAF} & 4
\end{array}
\]

(5.24)

giving the NCDAF approach a 25% advantage in speed. A second example,

\[
\begin{array}{ccc}
\text{elements} & \text{recursions} \\
M = 74 \text{ NCDAF} & 2775 & 73 \\
M = 53 \text{ CPDAF} & 2809 & 104
\end{array}
\]

(5.25)

shows a 30% advantage in speed. Other examples show a similar advantage of NCDAF over equivalent

\(^3\)Direct evaluation of higher order polynomials may increase the speed of the calculation but at the expense of decreased accuracy.
5.5 Approximation of Polynomials

A clear distinction between the CP and NCDAF approximations can be seen in the approximation of polynomials. Consider the polynomial depicted in figure 5.7 and detailed in appendix 5B. It is instructive to look at this polynomial in a term diagram

\[
\begin{array}{c}
\text{(i)} \\
0, 2, 4, 6, 8, 10, 12, 14 \\
\text{(j)} \\
0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 \\
\end{array}
\]

where a dot (•) indicates a term proportional to \(x_1^ix_2^j\). As demonstrated in chapter 4 [section 4.5.2] the 7th NCDAF approximation can exactly represent a 15 degree polynomial. This is confirmed in figure 5.8 for this example polynomial, where the residual for the 7th NCDAF is converged to machine precision.

These results of the NCDAF approximation are in strong contrast to those of the CPDAF method. Although the approximation of the equivalent 5th CPDAF approximation (which has 36 terms) is fairly good, as can be seen in figure 5.8, the error is orders of magnitude larger than the 7th NCDAF result. To achieve convergence to machine precision the 7th CPDAF approximation must be used (see figure 5.8).

The reason for these results can be explained by looking at the term diagrams. It should be noticed
that the term diagram for the 7th NCDAF,

![7th NCDAF Diagram](image)

matches the shape of that of the $P_{15}$ polynomial (eq. 5.26). More importantly, this NCDAF contains a term for each and everyone of the terms that transform as scalars of the $P_{15}$ polynomial. When the term diagram for the 5th CPDAF is examined

![5th CPDAF Diagram](image)

it is seen that it missing some of these scalar terms of the $P_{15}$ polynomial (e.g. $x_2^2x_1^2$). As can be seen
from the $7^{th}$ CPDAF term diagram,

\[ \text{7th CPDAF} \]

the missing contributions are included in this higher order approximation.

Now consider the example $22^{nd}$ degree polynomial depicted in figure 5.7 (see appendix 5B for details) with the following term diagram

\[ \text{P}_{22} \]

A quick review of the DAF term diagrams reveals this is a match for the $5^{th}$ CPDAF (eq. 5.28). Confirmation of this fact is demonstrated in figure 5.9 where it is seen the $5^{th}$ CPDAF approximation of the $P_{22}$ polynomial converges to machine precision. As can also been seen in the same figure, the equivalent $7^{th}$ NCDAF approximation is several orders of magnitude less accurate. To represent the $P_{22}$ polynomial to machine precision, the $10^{th}$ NCDAF approximation must be used.
The two example polynomials were chosen because they represent two possible extreme cases. The $P_{15}$ and $P_{22}$ polynomials contain 136 and 144 terms respectively making them similar in this regard. They differ in how these terms are distributed. The $P_{15}$ polynomial has more terms that couple $x_1$ and $x_2$ of largely different orders (e.g. $x_1^{13}x_2^2$) and the $P_{22}$ polynomial has more terms that couple $x_1$ and $x_2$ of close orders (e.g. $x_1^7x_2^8$). For an arbitrary polynomial one needs to determine if the term distribution is more like the $P_{15}$ (triangle) or $P_{22}$ (square) in order to decide which DAF method is the most suitable.

Although these conclusion are based upon approximating polynomials they should hold for more general functions. They are particularly useful for functions with essential features that can be well characterized in terms of polynomials over a region of interest.

### 5.6 Coordinate Axis Bias

In order to understand the coordinate axis bias of the CPDAF approximation it is useful to construct a function that has the same bias and may easily be rotated. With this in mind, consider the function

\[
f(x, y; \theta) = \exp \left( -2\omega_1 \left( \chi_1^2 + \chi_2^2 \right) \right) \cos (\omega_2 (\chi_1 + \chi_2)) \sin (\omega_2 (\chi_1 - \chi_2)) ,
\]

where

\[
\chi_1 = (x \cos \theta + y \sin \theta) ,
\]

\[
\chi_2 = (x \sin \theta - y \cos \theta) ,
\]

which is plotted in figure 5.10 for various values of $\theta$. When the value $\theta = \frac{\pi}{4}$ is used the various quantities take on the values

\[
\chi_1 \left( \frac{\pi}{4} \right) = \left( x \cos (\frac{\pi}{4}) + y \sin (\frac{\pi}{4}) \right) = \sqrt{\frac{1}{2}} (x + y) ,
\]

\[
\chi_2 \left( \frac{\pi}{4} \right) = \left( x \sin (\frac{\pi}{4}) - y \cos (\frac{\pi}{4}) \right) = \sqrt{\frac{1}{2}} (x - y) .
\]
\[
\chi_2\left(\frac{\pi}{4}\right) = \left( x \sin\left(\frac{\pi}{4}\right) - y \cos\left(\frac{\pi}{4}\right) \right) \quad (5.34\text{a})
\]
\[
= \sqrt{\frac{1}{2}} (x - y) \quad (5.34\text{b})
\]
\[
\chi_1\left(\frac{\pi}{4}\right) + \chi_2\left(\frac{\pi}{4}\right) = \sqrt{2x} \quad (5.35\text{a})
\]
\[
\chi_1\left(\frac{\pi}{4}\right) - \chi_2\left(\frac{\pi}{4}\right) = \sqrt{2y} \quad (5.35\text{b})
\]
\[
\chi_1^2 + \chi_2^2 = \frac{1}{2} (x^2 + 2xy + y^2) + \frac{1}{2} (x^2 - 2xy + y^2) \quad (5.36\text{a})
\]
\[
= x^2 + y^2 , \quad (5.36\text{b})
\]

Making the function

\[
f(x, y; \frac{\pi}{4}) = \exp\left(-\omega_1 \left(x^2 + y^2\right)\right) \cos(\omega_2x) \sin(\omega_2y) . \quad (5.37)
\]

Under such a rotation the axis bias of the function exactly coincides with the \(x-y\) axis of the CPDAF approximation

\[
\delta_{\text{CP}}(x', y'; M, \sigma) . \quad (5.38)
\]

Decreasing \(\theta\) results in an increasing mismatch of the axis with the greatest disparity occurring at \(\theta = 0\).

Now consider the CPDAF approximation of this function (eq. 5.31) for various orientations. In all the calculations the computational conditions were chosen to be fairly demanding; specifically, the sampling grid spacing was set to be near the DAF limit [see section 4.4] and values on and off the grid points were tested. The accuracy of the DAF was also chosen to be 5 to 6 decimal places with the optimal \(\sigma/\Delta\) parameters used [appendix 4C]. The effect of stepping \(\theta\) from \(\frac{\pi}{4}\) to 0 on the CPDAF approximation is depicted in figure 5.11. There is not only a dramatic qualitative change in the residual (error) but
the accuracy also drops by an order of magnitude. The CPDAF approximation is thus sensitive to the orientation of the function relative to its axis. For functions that have a distinct directional bias, as the example function used here does, the best orientation of the CPDAF axis is clear. For functions that are not so biased, one will have to resort to trial and error to find the best orientation.

The NCDAF approximation of this function (eq. 5.31) shows dramatically different results. From the residuals of the NCDAF approximation for the various cases of $\theta$, plotted in figure 5.12, it is seen that the effect is merely a rotation. The NCDAF is thus independent as to the choice of coordinate axis. It is therefore much simpler to implement than the CPDAF approximation, as one does not have to optimize the approximation by testing various rotations of the function being approximated.

5.7 Induced Artificial Rectangular Structure

One important advantage of the NCDAF over product methods is that it does not induce artificial rectangular structure into the approximation of the function. This can be demonstrated by considering the example function

$$f(x, y) = \cos(100x) + \cos \left(100(x \cos \left(\frac{\pi}{8}\right) + y \sin \left(\frac{\pi}{8}\right))\right)$$

$$+ \cos \left(100(x \cos \left(\frac{\pi}{4}\right) + y \sin \left(\frac{\pi}{4}\right))\right) + \cos \left(100(x \cos \left(\frac{3\pi}{8}\right) + y \sin \left(\frac{3\pi}{8}\right))\right)$$

$$+ \cos(100y) + \cos \left(100(x \cos \left(\frac{5\pi}{8}\right) + y \sin \left(\frac{5\pi}{8}\right))\right)$$

$$+ \cos \left(100(x \cos \left(\frac{7\pi}{8}\right) + y \sin \left(\frac{7\pi}{8}\right))\right) + 9 , \quad (5.39)$$

which is not a Cartesian product of one-dimensional functions. The NCDAF approximation of this function is show in figure 5.13. It should be noted that the error of the approximation looks very much like the function itself. This is consistent with the properties of the residual suggested by the non-rigorous analysis in section 4.5.3. An equivalent CPDAF approximation of the function is shown in figure 5.14. Although the approximation of the function is qualitatively very good, the residual clearly shows a square structure that is not present in original data.
The reason for this difference is due to a basic property of Cartesian products. In the momentum domain all such product methods have a rectangular shape. For data that have similar rectangular structures this may be an advantage, but for functions such as the above example it leads to an artificial bias. This can be seen in figure 5.15 which depicts the overlap of function 5.39 and the CPDAF in the momentum domain. It should be noted that all 16 components in the example function are equivalent (equal distance from the origin). The components of function that fall at the corners of the CPDAF plateau (e.g. \( k_x, k_y = \sqrt{\frac{1}{2}}, \sqrt{\frac{1}{2}} \)) are closer to unity than those at the edges (e.g. \( k_x, k_y = 1, 0 \)). This means that the CPDAF approximation significantly favors those contributions making them artificially different than the rest. The rectangular structure in the error (figure 5.14) is an obvious consequence of this bias.

From figure 5.15 it can be seen that the components of function 5.39 that lie along the diagonals in the momentum domain are actually slightly further from unity than for the CPDAF case; however, the ones that lie along the axis are much closer to unity. As a matter of fact all the components are approximated to the same degree of accuracy thus retaining their equivalence. This means the NCDAF does not impose a rectangular bias into the data.
Appendix 5A: Derivation of the Basic NCDAF and CPDAF Interrelationships

In this appendix the basic interrelationships of the NCDAF and the CPDAF are derived. Attention will be restricted to two dimensions and where the CPDAF can be characterized by a single $M$ and $a$.

Write the $M^{th}$ CPDAF kernel in the momentum domain,

$$
\tilde{\Delta}_{CP}(k_x, k_y; M, \sigma) = \sum_{n=0}^{M} \sum_{m=0}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right), \quad (5A.1)
$$

in two parts as

$$
\tilde{\Delta}_{CP}(k_x, k_y; M, \sigma) = \sum_{n=0}^{n+m=M} \sum_{m=0}^{n+m=M} \frac{1}{n!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) + \sum_{n=1}^{M} \sum_{m=M-n+1}^{M} \frac{1}{n!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right), \quad (5A.2)
$$

The first part can be rewritten by using the multinomial series [124],

$$
\sum_{N=0}^{M} \frac{1}{N!} \sum_{n,m} \frac{N!}{n! m!} a_1^n a_2^m = \sum_{N=0}^{M} \frac{1}{N!} (a_1 + a_2)^N, \quad (5A.4)
$$

to give

$$
\sum_{n=0}^{n+m=M} \sum_{m=0}^{n+m=M} \frac{1}{n!} \frac{1}{m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) = \sum_{N=0}^{M} \frac{1}{N!} \left( \frac{\sigma^2 (k_x^2 + k_y^2)}{2} \right)^N \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right), \quad (5A.5)
$$

This quantity should be recognized as the $M^{th}$ NCDAF Kernel,

$$
\tilde{\Delta}_{NC}(k_x, k_y; M, \sigma) = \sum_{N=0}^{M} \frac{1}{N!} \left( \frac{\sigma^2 (k_x^2 + k_y^2)}{2} \right)^N \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right), \quad (5A.6)
$$
The expression for the CPDAF in terms of the NCDAF kernel is thus

$$\tilde{\Delta}_{CP}(k_x, k_y; M, \sigma) = \tilde{\Delta}_{NC}(k_x, k_y; M, \sigma) \quad \text{(5A.7)}$$

$$+ \sum_{n=1}^{M} \sum_{m=M-n+1}^{M} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right)$$

Rewrite the $2M^{th}$ NCDAF kernel in the momentum domain,

$$\tilde{\Delta}_{NC}(k_x, k_y; 2M, \sigma) = \sum_{N=0}^{2M} \frac{1}{N!} \left( \frac{\sigma^2 (k_x^2 + k_y^2)}{2} \right)^N \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) \quad \text{(5A.8)}$$

by using the multinomial series

$$\tilde{\Delta}_{NC}(k_x, k_y; 2M, \sigma) = \sum_{n=0}^{2M} \sum_{m=0}^{2M} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) \quad \text{(5A.9)}$$

Divide this expression into three parts

$$\tilde{\Delta}_{NC}(k_x, k_y; 2M, \sigma) = \sum_{n=0}^{M} \sum_{m=0}^{M} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) \quad \text{(5A.10)}$$

$$+ \sum_{n=M}^{2M} \sum_{m=M-n+1}^{M} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right)$$

$$+ \sum_{m=0}^{2M} \sum_{n=0}^{2M-m} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right)$$

The first part should be recognized as the $M^{th}$ CPDAF kernel

$$\tilde{\Delta}_{CP}(k_x, k_y; M, \sigma) = \sum_{n=0}^{M} \sum_{m=0}^{M} \frac{1}{n! m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) \quad \text{(5A.11)}$$
The expression for the CPDAF in terms of the NCDAF kernel is thus

\[
\hat{\Delta}_{NC}(k_x, k_y; 2M, \sigma) = \hat{\Delta}_{CP}(k_x, k_y; M, \sigma) \\
+ \sum_{n=0}^{M-1} \sum_{m=M+1}^{2M-n} \frac{1}{n!} \left( \frac{\sigma^2 k_x^2}{2} \right)^n \frac{1}{m!} \left( \frac{\sigma^2 k_y^2}{2} \right)^m \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right) \\
+ \sum_{m=0}^{M-1} \sum_{n=M+1}^{2M-m} \frac{1}{m!} \left( \frac{\sigma^2 k_x^2}{2} \right)^m \frac{1}{n!} \left( \frac{\sigma^2 k_y^2}{2} \right)^n \exp \left( -\frac{\sigma^2}{2} (k_x^2 + k_y^2) \right)
\]

(5A.12)
Appendix 5B: Two Dimensional Test Polynomials

The 2D polynomials used for testing the DAF approximations in this chapter are of the same type used in chapter 4,

\[ P_n(x, y) = \frac{1}{\sum_{i=0}^{n} |c_i|} \sum_{i=0}^{n} c_i T_{m_i,i}^{\alpha_i, \beta_i}, \]  

(5B.1)

where the reader is referred to appendix 4B for details. The parameters for the 15\textsuperscript{th} degree polynomial are

<table>
<thead>
<tr>
<th>( i )</th>
<th>( c_i )</th>
<th>( \alpha_i )</th>
<th>( \beta_i )</th>
<th>( m_i )</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>-75</td>
<td>1</td>
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<td>7</td>
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<tr>
<td>1</td>
<td>100</td>
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<td>15</td>
<td>-100</td>
<td>5</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

(5B.2)
The parameters the 22\textsuperscript{nd} degree polynomial are

\begin{tabular}{cccc}
\(i\) & \(c_i\) & \(\alpha_i\) & \(\beta_i\) & \(m_i\) \\
0 & -75 & 1 & 1 & 11 \\
1 & 100 & 1 & 2 & 10 \\
2 & 20 & 3 & 1 & 9 \\
3 & -50 & 2 & 5 & 8 \\
4 & 35 & 5 & -2 & 7 \\
5 & -50 & 7 & 3 & 6 \\
6 & -15 & 3 & 2 & 5 \\
7 & 25 & 5 & -3 & 4 \\
8 & 50 & 1 & -1 & 3 \\
9 & -40 & 2 & 1 & 2 \\
10 & -50 & 7 & -2 & 1 \\
11 & 25 & 7 & 1 & 0 \\
\end{tabular}

(5B.3)
Figure 5.1: The NCDAF and CPDAF kernel in the position domain.
Figure 5.2: The NCDAF and CPDAF kernel in the momentum domain.
Figure 5.3: Demonstration that the $6^{th}$ NCDAF completely bounds the $3^{rd}$ CPDAF.
Figure 5.4: Demonstration that the 4th CPDAF completely bounds the 4th NCDAF.
Figure 5.5: Comparison of the 4th NCDAF and 3rd CPDAF
Figure 5.6: Example of how a DAF momentum window can bound at the top of the plateau but be exceeded at the foot of the cliff. Parameters used are $M = 2$ and $\sigma = 1.0$ (solid), and $M = 40$ and $\sigma = 4.0$ (dashed).
Figure 5.7: Test polynomials detailed in Appendix 5B.
Figure 5.8: Residuals for approximation of the $P_{15}$ polynomial.
Figure 5.9: Residuals for approximation of the $P_{22}$ polynomial.
Figure 5.10: Function 5.31 for various rotations.
Figure 5.11: Residual of the CPDAF approximation with $M = 8$ and $\sigma/\Delta = 1.75$ for various rotations of function 5.31.
Figure 5.12: Residual of the NCDAF approximation with $M = 9$ and $\sigma/\Delta = 1.65$ for various rotations of function 5.31.
Figure 5.13: NCDAF approximation with \((M = 5 \text{ and } \sigma/\Delta = 1.58)\). (a) function 5.39, (b) NCDAF approximation, (c) error, and (d) relative error.
Figure 5.14: CPDAF approximation (with $M = 4$ and $\sigma/\Delta = 1.56$). (a) function 5.39, (b) CPDAF approximation, (c) error, and (d) relative error.
Figure 5.15: Overlap of function 5.39 (‘x’s) with the CPDAF (left hand side, with \( M = 4 \) and \( \sigma/\Delta = 1.56 \)) and the NCDAF (right hand side, with \( M = 5 \) and \( \sigma/\Delta = 1.58 \)) in the momentum domain.
6 Constructing Missing Data with Non-Cartesian Distributed Approximating Functionals

Often investigators are faced with less data than desired. In experimental studies, data may be missing due to instrument failure. In theoretical studies, data can be limited by availability of computer resources. Estimation of the underlying phenomenon where data is unavailable can be advantageous. It can save time, effort, and other resources. For example consider the process of locating special points such as minima on potential energy surfaces. Each missing data point may require a considerable amount of computational expenditure to evaluate. Searches through gaps in the data, especially in multi-dimensions, can be too costly to be practical. In such a case, a rough estimate of the location of the points of interests is enough to be enormously helpful.

A particularly challenging situation is when the gap in the data is large compared to the Nyquist wavelength of the known data. For example, consider the data depicted in the following diagram.

![Diagram](image)

It appears that the function within the data gap contains a few complete oscillations. One method that can provide an accurate prediction of the underlying function in such a gap is the DAF data augmentation method [30][125][126]. This can be seen from the DAF prediction based on the above
This chapter presents the NCDAF generalization of the DAF data augmentation method. In the first section the basic principles of the NCDAF data augmentation method are discussed. The derivation of the method is then given in the second section. A number of issues concerning the implementation of this method are also discussed. In the last section some example calculations are given.

6.1 Basic Principles

A good estimation of a function in an unknown region should match with the boundary of known data smoothly. Mathematically this means that the function and as many of its derivatives as possible are continuous across the join. Assuming the derivatives are known, the function in an unknown region can be found by systematically varying the approximation to minimize discontinuities. The more complicated the function in the unknown gap, the higher the order of derivatives that are required for a good approximation. Higher order derivative values at the join, however, are not trivial to obtain. Estimations of derivatives near the edge are also often poor because they approach the derivative from only one direction (known data towards unknown gap). The NCDAFs provide a way to overcome this difficulty. The usefulness of the NCDAF is rooted in its property of holding the accuracy of the
derivatives on equal footing to the accuracy of the function approximation. For a well-tempered NCDAF approximation [sections 4.5.4 and 4.6] a good derivative fit is a natural consequence of a good function fit. This greatly simplifies the formulations as the predicted function in the gap needs to be varied with respect to minimizing the function error.

The NCDAF quantity that is a useful measure of the quality of fit is the cost function [section 4.5.1],

\[
Cost = \sum_i w_i |\tilde{g}_i - g_i|^2 ,
\]

(6.1)

where \(w_i\) are weights and \(\tilde{g}_i\) is the NCDAF approximation of the function \(g_i\) at the \(i^{th}\) point. The presence of the weights is to 1) define limits on the summation to prevent it from diverging, and 2) allow points which are considered more important to contribute more than other points. Since the primary interest is how good the approximation is at and near the join, let \(i\) be limited to points in the unknown gap and a few points that surround it on all sides. Obviously, the better the NCDAF approximation the smaller the cost function will be. It is important to point out that the sensitivity of the NCDAF approximation to discontinuities in the function and derivatives [section 4.5.7] is reflected in this cost function. The worse the join the higher the cost function will be.

Constructing missing data in large gaps with the NCDAF relies on finding the approximation that minimizes the cost function. The method starts with choosing a trial function with several parameters that may be varied. The least square procedure can then produce the set of values for the parameters that minimize the cost function.

It is often convenient to use a basis set for the trial function. The cost function then can be minimized with respect to varying the value of the coefficients of the basis set. Almost all choices of basis function require at least some crude idea of what the missing sections of the function looks like. The only basis function that is completely neutral to the particulars of the problem is a grid basis. This system uses a Kronecker delta, \(\delta_{ij}\), at each grid point as basis functions. Although derivations involving general basis functions are possible, only grid basis functions will be used in here.
6.2 Equations

6.2.1 Derivation

Consider sampling of a multidimensional function with large gaps of unsampled data. The function is divided into two regions: the known region consisting of sampled points, and the unknown region consisting of unknown points. It should be noted the unknown region may actually be several disconnected gaps in the data (see example calculation of image data below). A crucial assumption is that all the unknown points fall well within the outer boundary of the known region (see appendix 6A for alternative situations).

Starting by writing out the details of the cost function

\[ \text{Cost} = \sum_i w_i |\tilde{g}_i - g_i|^2 \]

(6.2a)

\[ = \sum_i w_i \left( \sum_j \left( \delta_{ij} - \delta_{ij} \right) g_j \right)^2 \]

(6.2b)

\[ = \sum_i w_i \sum_k \sum_j \left( \delta_{ki} - \delta_{ki} \right) \left( \delta_{ij} - \delta_{ij} \right) g_k g_j , \]

(6.2c)

where the \( i \) and \( j \) indices run over all points (known and unknown), \( \delta_{ij} \) is the \( i,j^{th} \) element of the NCDAF matrix (with the quadrature weight of \( j \)th point incorporated), and \( \delta_{ij} \) is the Kronecker delta.

Now denoting the value of the function at point \( a \) as \( g_a \), minimize by taking the derivative \( \frac{\partial}{\partial g_a} \),

\[ 0 = 2 \sum_i w_i \sum_j \left( \tilde{\delta}_{ai} - \delta_{ai} \right) \left( \tilde{\delta}_{ij} - \delta_{ij} \right) g_j , \]

(6.3)

resulting in

\[ 0 = \sum_j \left[ \sum_i w_i \left( \tilde{\delta}_{ai} - \delta_{ai} \right) \left( \tilde{\delta}_{ij} - \delta_{ij} \right) \right] g_j , \]

(6.4)
for each of the \( a \) unknown points. Regrouping the terms over known and unknown points gives

\[
- \sum_{m}^{\text{known}} \left[ \sum_{i} w_{i} (\delta_{ai} - \delta_{ai}) (\delta_{im} - \delta_{im}) \right] g_{m} = \sum_{b}^{\text{unknown}} \left[ \sum_{i} w_{i} (\delta_{ai} - \delta_{ai}) (\delta_{ib} - \delta_{ib}) \right] g_{b},
\]

(6.5)

where points over known region are indexed by \( m \), unknown region by \( a \) and \( b \). Defining

\[
h_{a} = - \sum_{m}^{\text{known}} \sum_{i} w_{i} (\delta_{ai} - \delta_{ai}) (\delta_{im} - \delta_{im}),
\]

(6.6)

and

\[
U_{ab} = \sum_{i} w_{i} (\delta_{ai} - \delta_{ai}) (\delta_{ib} - \delta_{ib}),
\]

(6.7)

allows the equation to be written in the matrix form

\[
h_{a} = \sum_{b}^{\text{unknown}} U_{ab} g_{b}
\]

(6.8)

\[
h = U g
\]

(6.9)

where bold capital letters are used for matrices and bold lower case letters for vectors. Solving for the value of the unknown points leads to

\[
U^{-1} h = g
\]

(6.10)

### 6.2.2 Practical Considerations

In practice it is not desirable to explicitly invert matrix \( U \) in equation 6.10. Looking at its structure (equation 6.7) it can clearly be seen as the NCDAF approximation improves \( (\delta_{ij} \rightarrow \delta_{ij}) \) the matrix becomes more singular making inversion disastrous. One way around this problem is with LU decomposition of \( U \) with back-substitution of \( h \) [16, p34-40]. This is not foolproof, so the condition number of \( U \), which is a measure of how ill-conditioned (or singular) the matrix is [16, p53], should always be noted. Due to the near singular aspect, better results are obtained by using NCDAF parameters that
are not optimal. Caution need to be employed as such NCDAFs are not guaranteed to be well-tempered and may exhibit other problems.

For computational purposes it is convenient to divide the known region into three subregions depicted in this diagram

\[
\text{known (} w_i = 0, \text{dof } = 0) \\
\text{known (} w_i = 0, \text{dof } \neq 0) \\
\text{known (} w_i \neq 0) \\
\text{unknown}
\]

The first subregion contains known points where the weight function \( w_i \) is nonzero. It should be large enough to surround the unknown region with at least a few points. Taken together with the unknown region this subregion defines the summation limits for the \( i \) index in equations 6.6 and 6.7. The second subregion contains all the remaining known points that are no more than an NCDAF bandwidth away from any point in the first subregion. All known points beyond this range of the NCDAF bandwidth form the third subregion. Since their effective contribution is zero, there is no need to include them in the calculation. The first two subregions taken together thus define the effective summation limit on the \( m \) index of equation 6.6. It can be seen that a dominate factor on the number of known points that are required for a calculation is the effective bandwidth of the NCDAF. In multiple dimensions this can lead to an extremely large number of points. It is thus crucial to use as small of a NCDAF width parameter (\( \sigma \)) as possible. The need for a small NCDAF bandwidth needs to be balanced with the need for the NCDAF to reach into the unknown region. For good approximations the rule of thumb is the magnitude of the NCDAF kernel should be appreciable half way into the unknown gap.

Addressing all of the above concerns makes using the NCDAF for constructing missing data a real balancing act. Often several combinations of parameters need to be tried until a result that looks qualitatively correct is obtained. There are however a few quantitative indicators of a good
approximation: 1) the condition number of the U matrix should be small but several orders of magnitude larger than an effective zero (e.g. $1 \times 10^{-16}$ for double precision), 2) the value of the cost function should be small, and 3) varying the NCDAF $\sigma$ parameter by a small amount should not cause a dramatic change in the prediction.

One of the simplest choices of weight functions is to set $w_i = 1$ for points in the unknown region and nearby sampled points, and $w_i = 0$ for all other distant points. Experience has shown that this rectangular weight function is suitable for many applications. More complicated shapes for the weight function are possible, but the advantages of doing so are left to future studies.

It is instructive to consider some limitations of the data augmentation method. One basic assumption of this method is that the actual function is infinitely smooth (differentiable to all orders). When this is not true the prediction in the unknown gap will be very poor. Consider for example the function

$$f(x) = \begin{cases} \exp(-\frac{1}{200} (x - 3)^2) (\sin(\frac{3}{4}x) + x + 2) & x < 3 \\ \exp(-\frac{1}{200} (x - 3)^2) (\sin(\frac{3}{4}x) + x - 8) & x \geq 3 \end{cases},$$

which is discontinuous at $x = 3$. The NCDAF prediction of this function with a gap between $x = [-4, 10]$ is plotted in figure 6.1, which as expected deviates significantly from the actual function. This represents an important inherent limitation of the NCDAF prediction method. It should also be noted that discontinuities in the function or derivatives in the known region near unknown regions are also likely to cause difficulties. As a second example consider the function

$$f_1(x) = \begin{cases} \sin(\frac{1}{2}x) & x < -3 \text{ or } x > 9 \\ \sin(\frac{1}{2}x) + \frac{1}{6} \sqrt{36 - (x - 3)^2} & -3 \leq x \leq 9 \end{cases},$$

with a gap between $x = [-4, 10]$. In this case the function is continuous but it contains a non-analytic feature which is completely limited to inside the unknown gap. As can be seen in figures 6.2a and 6.2b, the NCDAF data augmentation is totally ignorant of this feature.
Another limitation is related to the accuracy of the method. Consider the example function

\[ f_2(x) = \sin\left(\frac{1}{2}x\right) + \exp\left(-\frac{1}{2} (x - 6.25)^2\right), \quad (6.14) \]

again with a gap between \( x = [-4, 10] \). In this case, the magnitude of the Gaussian feature is relatively insignificant outside the gap. From figures 6.2c and 6.2d it is seen the influence of the feature is below the level of accuracy of the prediction. In contrast, the influence of the Gaussian feature of function

\[ f_3(x) = \sin\left(\frac{1}{2}x\right) + \exp\left(-\frac{1}{72} (x - 3)^2\right), \quad (6.15) \]

is above the level of accuracy of the data augmentation method, as can be seen in figure 6.2e.

### 6.3 Example Calculations

#### 6.3.1 One-Dimensional Example

The first example calculation is a recreation of the one from publication [30]. Consider the one-dimensional function

\[ f(x) = 5 \exp(- (x - 1)^2) + 2 (\cos(x) + \cos(2x) + \cos(3x) + \cos(4x)) + 4, \quad (6.16) \]

with a gap from \( x = -1.87 \) to 1.87. It should be noted that this gap is several time larger than the function's minimum wavelength (which is about 0.7854) making this test a particularly challenging one. The known function is sampled with the spacing of \( \Delta x = 0.09828 \) with a unity weight function from \( x = -50 \Delta x \) to \(-20 \Delta x\) and \( x = 20 \Delta x \) to \( 50 \Delta x \). This leaves a gap in the data that is 39 points.

The result of the NCDAF prediction with \( M = 40 \) and \( \sigma/\Delta = 8.75 \) (\( \sigma \approx 0.9 \)) is plotted in figure 6.3. Qualitatively the prediction is a perfect match with no noticeable differences. The quantitative differences are detailed in table 6.1. Given the complexity of the missing segment the error of 0.2% or less is remarkable. This example also illustrates the general behavior of the error; that is, the error is
small near the edges of the gap and progressively gets larger as the center of the gap is approached. The error is also responsive to the characteristics of the function. It follows the trend that the NCDAF approximation is poorest at extrema and best at inflection points (where the second derivative vanishes) [22]. This can be seen in table 6.1 as the maximum error occurs at $-9\Delta x$, which is near a minimum in the function, instead of at the center of the gap.

These results are consistent with those of the original method used in the previous publication [30]. The notable difference is that the NCDAF data augmentation method can produce results a factor of 10 better with 4 times fewer sampled known points.

### 6.3.2 Two Dimensional Example

The NCDAF prediction method easily generalizes to more than one dimension as this second example illustrates. Consider the two dimensional function

$$f(x,y) = \exp\left(-\frac{1}{200} R_a^2\right) \sin\left(\frac{7}{4} R_a\right) + \exp\left(-\frac{1}{50} R_b^2\right) \cos(2R_b) + \exp\left(-\frac{1}{150} R_c^2\right) \sin\left(\frac{5}{4} R_c\right) + 4, \quad (6.17)$$

where

$$R_a = \sqrt{(x-10)^2 + (y-15)^2}$$

$$R_b = \sqrt{(x-12)^2 + (y-12)^2}$$

$$R_c = \sqrt{(x-23)^2 + (y-19)^2}$$

(6.18)

with a square gap in the data over the range $x = [10, 14]$ and $y = [10, 14]$. The function minus the unknown gap is plotted in figure 6.4a. It should be noted that the gap is a few times larger than the minimum wavelength of this function (which is about 1.57). Although this problem should be less challenging than the previous example, the goal will only be to produce qualitative results. The known region is sampled with the spacing $\Delta x = \Delta y = 0.2$ with a unity weight function over the range that falls within the radius of 5 of the unknown region. It should be noted that the gap is 20 points along each dimension make a total of 400 unknown points.
The resulting prediction for \( M = 11 \) and \( \sigma/\Delta = 4.75 \ (\sigma \approx 0.95) \) is plotted in figure 6.4b (and 6.5a) which is a good qualitative match for the actual function plotted in figure 6.5b. All the essential characteristics, such as extrema, are predicted to lie very close to their true locations. Like the one-dimensional case the error is a function of the distance from known points and the characteristics of the function. As can be seen in figures 6.5c and d, there is general increase in error towards the center of the unknown gap. It can also be seen that the largest errors occur near a saddle point (roughly centered at point 6,14 on the error plots) and the maximum (roughly centered at point 11,8). In the percent error (figure 6.5d) there is a distinctive improvement in prediction’s accuracy midway between the extrema where an inflection line should fall. In more than one dimension there is another factor effecting the accuracy of the prediction; that is, the number of known points near an unknown point. The more known points within a given radius of the unknown point the better the prediction should be. For example, the unknown points near corners of a gap should have smaller errors than points elsewhere that are at similar distances to the nearest known point. This is seen in the example calculation (see figures 6.5c and d) as better approximation at the corners leads to the overall circular shape of the error (despite the fact the gap is square in shape).

6.3.3 Image Example

A field of enormous potential application of the NCDAF data augmentation method is image restoration. The primary reason is that image restoration only requires the results to be only visually accurate. Even under difficult conditions experience has shown the NCDAF can provide qualitative results. Image data, however, possesses its own set of challenges. A typical commercially available digital camera may have an intensity depth as little as 256. Differences of just one intensity unit (about 0.4%) are near the perceptual limit. This fact, taken with the experience that the NCDAF prediction is usually several orders of magnitude less accurate than the known data, means even a qualitative result can be challenging. It should be noted as advanced technology becomes more affordable this difficulty will be mitigated to a large extent. A more profound difficulty is that image data is full of discontinuities.
Every edge of an object in an image is a discontinuity. Unfortunately, the DAF data augmentation procedure is likely to either blur the edges (as in figure 6.1) or lead to ringing (the image analysis terminology for Gibbs phenomena). The challenge is to make these errors as unnoticeable as possible.

The damaged image that will be used for an example calculation can be found in figure 6.6a. The type of damage is known as impulse (or shot noise) [127] where isolated points either take on random values or are missing. It is most often the result of damaged pixels in a camera, but it could also model very tiny defects or dirt on a photograph. It should be noted that this is one of the easiest types of defects to remove and thus serves as an elementary test of any image restoration method. The particular image used is 128 by 128 pixels and each pixel has an intensity range of 0 to 255. It should be noted that the image contains some relatively detailed features such as hair and a mix of gravel and dirt in the background.

In order to maximize isolation, the 256 bad points are laid out quasi-randomly using a Sobol's sequence [16, p299-304]. To avoid the issue of how to treat the edges (see appendix 6A) all the shot noise was placed far from the edge of the image. For convenience it will be assumed the location of the shot noise is known. The weight function used was simply unity at the unknown points and the eight surrounding points. It should be noted that the level of impulse noise in this example is relatively low (about 3%). In a more realistic application as much as 40% of the pixels can be bad. To extend this method to such cases an iterative procedure can be used (see reference [128] for example). This example thus represents what is practical to do in one iteration with limited computational resources.

Figure 6.6b shows the NCDAF restored image (with $M = 11$ and $\sigma = 2.5$). The original undamaged image is shown in figure 6.6d for comparison. Though there are perceptible differences, no feature in the restored image looks wrong when viewed by itself. The maximum quantitative error was just under 12% with the average being around 2%. Figure 6.6c shows the spatial location of the larger errors. As expected the largest errors tend to occur at sharply focused edges and detailed areas such as the hair.
Appendix 6A: Edge Treatments and Extrapolation

The method described in this chapter is limited to cases where the unknown gap in the data is surrounded by known data. There are, however, a number of cases where it is desirable to approximate data that is at the edge or outside the boundaries of known data. It is also possible for an unknown region to fall totally within the bounds of the known data but too near the edge for an accurate calculations (recall that the unknown data needs to be surrounded by a NCDAF bandwidth of data on all sides).

Difficulties associated with not knowing the function outside the a finite region is not limited to just the NCDAF data augmentation method. Consider trying to take the Fourier transform a function that is neither periodic nor completely localized in the known region. Without a strategy for treating the edges the approximation is likely to be extremely poor. Various elementary schemes exist for padding the edges of data known in only a finite region. A couple example treatments are depicted in figure 6.7. Other possibilities include attaching a function to the boundaries of the known data that smoothly attenuates to zero. This treatment has the associated problem of exactly how to choose the smoothly attenuating function.

A clever padding scheme that uses the principles of the main chapter is described in references [125][126]. Basically, the non-periodic data is taken to be periodic with an small gap of unknown points joining opposite ends of the data. It is then a simple matter to predict the values in the unknown gap to create data which is periodic. It is important to note this was done in the publication as 1D strips of data. As of this time there is no NCDAF implementation of this method.

Two other generalization of the NCDAF data augmentation method are presented in this appendix. The first uses basis functions to represent the function on the sides opposite the known data. The coefficients of the basis functions then are varied along with the value of points between the known and basis function regions. An alternative generalization [125] periodically repeats the unknown points outward from the edge of the known region. Both generalization help stabilize the extrapolation by tying down the external edge of the unknown region. For simplicity it will be assumed the unknown
region is entirely at the outside edge of the known data. It will be left up to the reader to make the
generalization to unknown regions that lie within the boundaries but near the edge of the known data.

6A.1 Basic Function Tail

Consider a set of data which can be divided into a known region and an unknown region which falls
outside the boundaries of the known region but shares at least one edge. The unknown region is then
to be further divided into a region of unknown values at grid points and unknown coefficients of basis
functions. These two unknown regions are arranged so the unknown points are surrounded by the
known and basis function regions. Pictorially this can be summarized by

\[
\text{indices} \quad m \ n \ a \ b \ c \ \alpha \ \beta
\]

\[
daf \neq 0
\]

\[
w_i \neq 0
\]

which for clarity is represented in one dimension. For future reference the range the weight function
and DAF are non-zero are also depicted.

It is convenient to start from a cost function which is divided up into the three regions

\[
\text{Cost} = \sum_{i} w_i \left( \sum_{m} (\delta_{im} - \delta_{im}) g_m + \sum_{b} (\delta_{ib} - \delta_{ib}) g_b + \sum_{\mu} \sum_{\beta} (\delta_{i\beta} - \delta_{i\beta}) \phi_{\mu}(z_{\beta}) \gamma_{\mu} \right) ^2
\]

where \( \phi_{\mu} \) are the \( N \) basis functions with \( \gamma_{\mu} \) coefficients, the index \( m \) runs over the region of known
points, index \( b \) (\( a \) and \( c \)) runs over the region of unknown points, and index \( \beta \) (and \( \alpha \)) over the region
containing the basis functions. The goal is to minimize this cost function with respect to value at the
unknown grid points and the coefficients of the basis functions.
First take the partial derivative with respect to the value at the unknown grid points,

$$0 = 2 \sum_{i} w_i \left( \sum_{c} \left( \delta_{ic} - \delta_{ic} \right) \left( \frac{\partial}{\partial g_{i}} g_{c} \right) \left( \sum_{m} \left( \delta_{im} - \delta_{im} \right) g_{m} + \sum_{b} \left( \delta_{ib} - \delta_{ib} \right) g_{b} \right) + \sum_{\mu} \sum_{\beta} \left( \delta_{i\beta} - \delta_{i\beta} \right) \phi_{\mu}(x_{\beta}) \gamma_{\mu} \right) \right), \quad (6A.3)$$

resulting in

$$0 = \sum_{i} w_{i} \left( \sum_{m} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{im} - \delta_{im} \right) g_{m} + \sum_{b} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{ib} - \delta_{ib} \right) g_{b} \right) + \sum_{\mu} \sum_{\beta} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{i\beta} - \delta_{i\beta} \right) \phi_{\mu}(x_{\beta}) \gamma_{\mu} \right), \quad (6A.4)$$

for each of the a unknown points. The equation now needs to be rearranged,

$$- \sum_{i} w_{i} \sum_{m} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{im} - \delta_{im} \right) g_{m} = \sum_{i} w_{i} \sum_{b} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{ib} - \delta_{ib} \right) g_{b} + \sum_{i} w_{i} \sum_{\mu} \sum_{\beta} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{i\beta} - \delta_{i\beta} \right) \phi_{\mu}(x_{\beta}) \gamma_{\mu} \right), \quad (6A.5)$$

to separates out the terms which just involve known quantities. It convenient to designate

$$h_{a} = - \sum_{i} w_{i} \sum_{m} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{im} - \delta_{im} \right) g_{m} \quad (6A.6)$$

and

$$U_{ab} = \sum_{i} w_{i} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{ib} - \delta_{ib} \right), \quad (6A.7)$$

$$U_{a\mu} = \sum_{i} w_{i} \sum_{\mu} \sum_{\beta} \left( \delta_{ia} - \delta_{ia} \right) \left( \delta_{i\beta} - \delta_{i\beta} \right) \phi_{\mu}(x_{\beta})$$
which allow the above equation to be written as

$$h_a = \sum_{b}^\text{unknown points} U_{ab}g_b + \sum_{\mu}^N U_{\alpha\mu}\gamma_\mu \quad \text{(6A.8)}$$

Now consider taking the partial derivative of the cost function (eq. 6A.2) with respect to the coefficients of the basis functions,

$$0 = 2\sum_i^\text{all basis} w_i \left( \sum_{\alpha}^\text{unknown basis} (\delta_{i\alpha} - \delta_{i\beta}) \phi_{\lambda}(x_\alpha) \left( \frac{\partial}{\partial \gamma_\lambda} \right) \sum_{m}^\text{known basis} (\delta_{im} - \delta_{im}) g_m \right)$$

$$+ \sum_{b}^\text{unknown points} (\bar{\delta}_{ib} - \delta_{ib}) g_b + \sum_{\mu}^\text{unknown basis} \sum_{\beta}^\text{known basis} (\delta_{\beta \mu} - \delta_{ib}) \phi_{\mu}(x_\beta)\gamma_\mu \quad \text{(6A.9)}$$

resulting in

$$0 = \left( \sum_i^\text{all basis} w_i \sum_{\alpha}^\text{unknown basis} (\delta_{i\alpha} - \delta_{i\beta}) (\bar{\delta}_{im} - \delta_{im}) \phi_{\lambda}(x_\alpha) g_m + \sum_{b}^\text{unknown points} (\bar{\delta}_{ib} - \delta_{ib}) g_b \right)$$

$$+ \sum_i^\text{all basis} w_i \sum_{\alpha}^\text{unknown basis} \sum_{b}^\text{unknown points} (\delta_{i\alpha} - \delta_{i\beta}) (\delta_{ib} - \delta_{ib}) \phi_{\lambda}(x_\alpha)\phi_{\mu}(x_\beta)\gamma_\mu \quad \text{(6A.10)}$$

for each of the $\eta$ basis functions. Rearranging this equation results in

$$-\sum_i^\text{all basis} w_i \sum_{\alpha}^\text{unknown basis} (\delta_{i\alpha} - \delta_{i\beta}) (\bar{\delta}_{im} - \delta_{im}) \phi_{\lambda}(x_\alpha) g_m \quad \text{(6A.11)}$$

$$= \sum_i^\text{all basis} w_i \sum_{\alpha}^\text{unknown basis} \sum_{b}^\text{unknown points} (\delta_{i\alpha} - \delta_{i\beta}) (\bar{\delta}_{ib} - \delta_{ib}) \phi_{\lambda}(x_\alpha) g_b$$

$$+ \sum_i^\text{all basis} w_i \sum_{\alpha}^\text{unknown basis} \sum_{\beta}^\text{known basis} \sum_{\mu}^\text{unknown basis} (\delta_{i\alpha} - \delta_{i\beta}) (\delta_{ib} - \delta_{ib}) \phi_{\lambda}(x_\alpha)\phi_{\mu}(x_\beta)\gamma_\mu \quad .$$
which can be written as

\[ h_\eta = \sum_b U_{qb} g_b + \sum_\mu U_{\eta \mu} \gamma_\mu, \]  

(6A.12)

where

\[ h_\eta = -\sum_i \sum_\alpha \sum_\beta \sum_m (\delta_{ia} - \delta_{i\alpha}) (\delta_{ib} - \delta_{i\beta}) \phi_\eta(x_\beta) g_\alpha, \]  

(6A.13)

and

\[ U_{qb} = \sum_i \sum_\alpha (\delta_{ia} - \delta_{i\alpha}) (\delta_{ib} - \delta_{i\beta}) \phi_\eta(x_\beta), \]

(6A.14)

\[ U_{\eta \mu} = \sum_i \sum_\alpha \sum_\beta (\delta_{i\alpha} - \delta_{i\beta}) (\delta_{i\beta} - \delta_{i\beta}) \phi_\eta(x_\beta) \phi_\mu(x_\beta). \]

The resulting equations (6A.8 and 6A.12) can be expressed in a matrix equation,

\[
\begin{pmatrix}
  h_a \\
  h_\eta
\end{pmatrix} =
\begin{pmatrix}
  U_{ab} & U_{a\mu} \\
  U_{\eta b} & U_{\eta \mu}
\end{pmatrix}
\begin{pmatrix}
  g_b \\
  \gamma_\mu
\end{pmatrix},
\]  

(6A.15)

where bold capital letters are used for matrices and bold lower case letters for vectors. The values at the unknown points and at the coefficients of the basis functions can then be solved by

\[ U^{-1} h = g. \]  

(6A.16)

6A.2 Periodic Tail

In this generalization of the DAF data augmentation method the unknown region of points will be taken to start at the edge of the known region and periodically repeat as they move outward. Since the details of the periodicity depend on the dimensionality, only the special case of one dimension will be
where the unknown points have a period of $p$ points. Note that although the diagram show the weight going to zero in the first repeat, the cut-off can be made at any point in the repeat region. In this method the presence of the weight function is crucial as the function in at least the direction of the periodic tail does not approach zero as the distance goes to infinity. The resulting summations without the cut-off imposed by the weight would be infinite.

To solve for the unknown points start from the familiar cost function

$$\text{Cost} = \sum_i \sum_j \left( \sum_k \left( \tilde{\delta}_{ki} - \delta_{ki} \right) g_j \right)^2$$

and minimize it with respect to varying the value at the unknown points. It is important to kept in mind that the value of the unknown point repeats itself every $p$ points. Start by taking the partial derivative with respect to the value at the unknown grid points which results in

$$0 = 2 \sum_i \sum_j \left( \sum_n \left( \tilde{\delta}_{a+n,p,i} - \delta_{a+n,p,i} \right) \right) \left( \tilde{\delta}_{ij} - \delta_{ij} \right) g_j$$

for each of the $a$ unique values of the unknown points. Moving the terms involving just known quantities
gives
\[
- \sum_m \left[ \sum_i w_i \left( \sum_{n=0}^{\infty} (\delta_{a+n,p,i} - \delta_{a+n,p,i}) \right) (\delta_{im} - \delta_{im}) \right] g_m \quad (6A.20)
\]
\[
= \sum_b \left[ \sum_i w_i \left( \sum_{n=0}^{\infty} (\delta_{a+n,p,i} - \delta_{a+n,p,i}) \right) (\delta_{ib} - \delta_{ib}) \right] g_b ,
\]
which can be written as
\[
h_a = \sum_b U_{ab} g_b ,
\]
(6A.21)
where
\[
h_a = - \sum_m \left[ \sum_i w_i \left( \sum_{n=0}^{\infty} (\delta_{a+n,p,i} - \delta_{a+n,p,i}) \right) (\delta_{im} - \delta_{im}) \right] g_m ,
\]
(6A.22)
and
\[
U_{ab} = \left[ \sum_i w_i \left( \sum_{n=0}^{\infty} (\delta_{a+n,p,i} - \delta_{a+n,p,i}) \right) (\delta_{ib} - \delta_{ib}) \right] .
\]
(6A.23)
In matrix form equation 6A.21 is
\[
h = Ug ,
\]
(6A.24)
which can be solved by
\[
U^{-1}h = g .
\]
(6A.25)
Figure 6.1: Function 6.12 (solid) with a gap taken between $x = [-4,10]$ and NCDAF approximation (diamonds) with $M = 13$ and $\sigma/\Delta = 3.00$. 
Figure 6.2: Limitation of the NCDAF data augmentation method towards localized features. NCDAF predictions are the diamonds for (a) function 6.13, (c) function 6.14, (e) function 6.15. (b) and (d) are the functions (a) & (c) minus the features.
Figure 6.3: Function 6.16 (solid) with a gap between $-19\Delta x$ and $19\Delta x$, and the NCDAF approximation with $M = 40$ and $\sigma/\Delta = 8.75$ (diamonds).
Figure 6.4: Function 6.17 (a) minus unknown gap, and (b) with the NCDAF approximation in unknown gap. Plots are in units of $\Delta x$ and $\Delta y$. 
Figure 6.5: (a) detail of the NCIDAF approximation in gap (b) actual function in gap, (c) absolute error, and (d) % error. Plots are in units of $\Delta x$ and $\Delta y$ with (c) & (d) shifted down by 50 units along both directions.
Figure 6.6: (a) image with shot noise, (b) NCDAF restored image, (c) % error, and (d) actual image.

Error scale darkest to lightest is greater than 9%, 7%, 5%, and 3%. All errors below 3% are not depicted.
Figure 6.7: A couple elementary examples of edge treatments: (a) the data is simply taken to be periodic (b) the data is reflected at the boundaries.
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<th>$x$</th>
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Table 6.1: error and % error in the NCDAF prediction of function 6.16 ($x$ is in units of $\Delta x$).
7 The Non-Cartesian Distributed Approximating Functional Representation of the Quantum Mechanical Free Evolution Propagator

The Time Dependent Schrödinger Equation (TDSE),

$$\frac{i\hbar}{\partial t}\psi(\vec{r};t) = \hat{H}\psi(\vec{r};t),$$

(7.1)

is an example of an initial value problem, where the states as a function of time are determined by the state at an initial time\(^1\). For time independent Hamiltonians (\(\hat{H}\)), it has the formal solution

$$\psi(\vec{r};t_0 + \Delta t) = \exp\left(-\frac{i\hat{H}\Delta t}{\hbar}\right)\psi(\vec{r};t_0),$$

(7.2)

where \(t_0\) is an initial time and \(\Delta t\) is a time interval. The operator

$$\exp\left(-\frac{i\hat{H}\Delta t}{\hbar}\right),$$

(7.3)

is called the propagator [4, p308-311][64] since it can be viewed as translating (in time) the initial state, \(\psi(\vec{r};t_0)\), into the state at a later time, \(\psi(\vec{r};t_0 + \Delta t)\), under the action of the Hamiltonian. This solution is formal as the construction of the propagator is equivalent to solving the TDSE explicitly [64]. A major advantage of TDSE methods is that the initial state need not be an eigenstate of the Hamiltonian. In fact the propagator is independent of any of the properties of the state being propagated.

Due to the fact that there is no representation in which the kinetic (\(\hat{K}\)) and potential energy (\(\hat{V}\)) parts of the Hamiltonian are simultaneously diagonal, it is convenient to separate them. This operator splitting of an exponential can only be done approximately because of the non-commuting of \(\hat{K}\) and \(\hat{V}\).

\(^1\)since TDSE permits time reversal, states at all previous times are also determined from an 'initial' state.
A commonly used example is the symmetric Trotter approximation [65][132]

\[
\exp \left( -i \frac{\hat{K} + \hat{V}}{\hbar} \Delta t \right) \approx \exp \left( -i \frac{\hat{V} \Delta t}{\hbar} \right) \exp \left( -i \frac{\hat{K} \Delta t}{\hbar} \right) \exp \left( -i \frac{\hat{V} \Delta t}{\hbar} \right) ,
\]

(7.4)

which is of second order accuracy in the time-step (\Delta t). If

\[
\Delta t = \frac{\text{total time}}{N} ,
\]

(7.5)

where \( N \) is the number of time-steps, then as \( N \to \infty \) this approximation becomes exact. By separating the propagator into parts that depend on \( \hat{K} \) and \( \hat{V} \), all the factors can be evaluated in the representation they are diagonal. The potential energy part can easily be evaluated in the position domain. The kinetic energy part of the propagator,

\[
\exp \left( -i \frac{\hat{K} \Delta t}{\hbar} \right) ,
\]

(7.6)

known as the free evolution propagator (FEP), is trivial to evaluate in the momentum domain. The attraction of this approach is that it can be made very efficient with Fast Fourier Transforms (FFT) [16, p490-529][122][133][134]. However, the position representation of this operator is computationally difficult to evaluate in the short time limit where equation 7.4 is valid. This can be seen in figure 7.1 where the FEP in the position domain for two relatively small time-steps are depicted.

In this chapter the NCDAF representation of the FEP is presented. The advantage of the NCDAF representation is that, unlike the exact FEP, it exhibits Gaussian dampening in the coordinate representation. This is more favorable for computational implementation. The effect of the FEP on the NCDAF kernel can be evaluated analytically. The consequence of this is that the only approximation involved is the NCDAF approximation of the initial state; that is, the NCDAF approximation of a function is propagated exactly.

In the first section of this chapter the properties of the FEP are discussed. Armed with insight into the exact FEP, the NCDAF FEP is derived in the second section. The third section is devoted
to numerical implementation. Since practical applications require the wavefunction to be represented as points on a discrete grid, the discretized expressions for the NCDAF FEP are derived. The added complications in choosing the optimal NCDAF parameters are then discussed. Since applications require several time-steps to be taken, the effect of repeat applications of the NCDAF is reviewed in the propagator context. In the last section, results from two calculations are given.

It should be mentioned that the NCDAF propagator method can be useful to other wave propagation problems. This methodology can apply to linear partial differential equations that are first order in the "progress" variable. Examples include the Helmholtz [135], the heat-diffusion [136], and the Bloch [137] equations. Equations that are second order in the progress variable may also be solved by two coupled propagations. A prominent example of this is the coupled propagator solution of the acoustic wave equation [138]. Good numerical results have even been achieved for nonlinear equations [139] such as the non-linear Schrödinger equation [43][140] and the Ginzburg-Landau equation [141] using generalizations of exponential propagation methods. In an appendix to this chapter, the NCDAF propagator of the heat-diffusion equation is derived as an example. In another appendix the results are generalized to the general class of operators known as metaplectic.

7.1 Free Evolution Propagator

Consider the TDSE for a system free of external potential, which is given by

$$\frac{\hbar}{2m} \frac{\partial}{\partial t} \psi(\vec{r}; t) = -\frac{\hbar^2}{2m} \nabla^2_{\vec{r}} \psi(\vec{r}; t) , \quad (7.7)$$

where $\vec{r}$ is the set of spatial coordinates, $t$ is the time parameter, $m$ is the mass, and $\nabla^2_{\vec{r}}$ is the Laplacian. The temporal derivative may be integrated,

$$\psi(\vec{r}; t_0 + \Delta t) = \frac{\hbar}{2m} \int_{t_0}^{t_0 + \Delta t} dt' \nabla^2_{\vec{r}} \psi(\vec{r}; t') + \psi(\vec{r}; t_0) , \quad (7.8)$$
yielding
\[ \psi(\vec{r}; t_0 + \Delta t) = \exp \left( \frac{i\hbar \Delta t}{2m} \nabla^2_{\vec{r}} \right) \psi(\vec{r}; t_0), \] \hspace{1cm} (7.9)

where \( \Delta t \) is a time interval and the exponentiated operator
\[ \rho_f(\nabla^2_{\vec{r}}; \Delta t) = \exp \left( \frac{i\hbar \Delta t}{2m} \nabla^2_{\vec{r}} \right) \] \hspace{1cm} (7.10)

is the free evolution propagator (FEP) [64]. The meaning of such an operator can be interpreted in terms of Taylor series
\[ \rho_f(\nabla^2_{\vec{r}}; \Delta t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ i \left( \frac{\hbar}{2m} \nabla^2_{\vec{r}} \right) \Delta t \right]^n, \] \hspace{1cm} (7.11)

where it should be noted that Laplacians of all orders are involved.

In the form of equation 7.9, the usefulness of the FEP is rather limited. Evaluation of an infinite order of Laplacians for an arbitrary initial state is impossible. Only a few special cases of initial states, such as plane waves
\[ \psi_{pw}(\vec{r}; \vec{k'}, t_0) = \left( \frac{1}{2\pi \hbar} \right)^{D/2} \exp \left( i \vec{r} \cdot \vec{k'} \right) \exp \left( \frac{i\hbar v_0 (k')^2}{2m} \right), \] \hspace{1cm} (7.12)

and Gaussian (Wavepacket) [142]
\[ \psi_{wp}(\vec{r}; \alpha, \vec{k}, \vec{k'}, t_0) = \left( \frac{1}{\pi \alpha^2} \right)^{D/4} \exp \left( -\frac{1}{2\alpha^2} (\vec{r} - \vec{r}_0)^2 \right) \exp \left( i \vec{r} \cdot \vec{k} \right) \exp \left( \frac{i\hbar v_0 (k_0)^2}{2m} \right), \] \hspace{1cm} (7.13)

can be evaluated in an analytic form. It will be useful for later results to evaluate the effect of the FEP on these two examples. To find the effect of the propagator on plane wave states,
\[ \rho_f(\nabla^2_{\vec{r}}; \Delta t) \psi_{pw}(\vec{r}; \vec{k'}, t_0) = \exp \left( \frac{i\hbar \Delta t}{2m} \nabla^2_{\vec{r}} \right) \exp \left( i \vec{r} \cdot \vec{k'} \right) \exp \left( \frac{i\hbar v_0 (k')^2}{2m} \right), \] \hspace{1cm} (7.14)
start by writing the Laplacian in its abstract operator form,

\[
\exp \left(-\frac{i\hbar \Delta t}{2m} \frac{1}{\hbar^2} \left(-\hbar^2 \nabla^2_r\right) \right) \exp \left(i \vec{r} \cdot \vec{k'}\right) = \exp \left(-\frac{i\hbar \Delta t}{2m} \frac{p^2}{\hbar^2} \right) \exp \left(i \vec{r} \cdot \vec{k'}\right) \quad (7.15a)
\]

\[
= \exp \left(-\frac{i\hbar \Delta t}{2m} \frac{\vec{k} \cdot \vec{k}}{\hbar^2} \right) \exp \left(i \vec{r} \cdot \vec{k'}\right) \quad (7.15b)
\]

Since plane waves are eigenstates of the momentum, the result is simply

\[
\psi_{pw}(\vec{r}; t_0 + \Delta t) = \exp \left(-\frac{i\hbar (t_0 + \Delta t)}{2m} \frac{k^2}{\hbar^2} \right) \exp \left(i \vec{r} \cdot \vec{k'}\right) . \quad (7.16)
\]

The effect of the FEP on a Gaussian,

\[
\rho_f(\nabla^2_r; \Delta t) \psi_{wp}(\vec{r}; \alpha, \vec{r}_0, \vec{k}_0, t_0) = \exp \left(-\frac{\Delta t}{2m} \nabla^2_r \right) \exp \left(-\frac{(\vec{r}_0 - \vec{r})^2}{2\alpha^2} + \frac{1}{\hbar} \vec{k}_0 \cdot \vec{r} + \frac{1}{2m} \frac{\hbar \omega(k_0)^2}{4} \right) , \quad (7.17)
\]

is given by [143, with \(\sqrt{2}\delta = \alpha\]

\[
\psi_{wp}(\vec{r}; t_0 + \Delta t) = \left(\frac{\alpha^2}{\alpha^2 + i\hbar \Delta t/m}\right)^{D/4} \exp \left(-\frac{(\vec{r} - \vec{r}_0 - \Delta t \vec{v}_0)^2}{2(\alpha^2 + i\hbar \Delta t/m)}\right) \exp \left(i \vec{k}_0 \cdot (\vec{r} - \vec{v}_0 \Delta t) + \frac{\hbar \omega(k_0)^2}{2m} \right) , \quad (7.18)
\]

where \(\alpha^2 = \alpha^2\), \(\vec{r}_0 = \langle \vec{r} \rangle_{t=0}\) is the initial average position, \(\vec{k}_0 = \langle \vec{p} \rangle_{t=0} / \hbar\) is the scaled (initial) group momentum, and \(\vec{v}_0 = \langle \vec{p} \rangle_0 / m\) is the classical velocity. Physically what is happening is that the center of the wavepacket is changing according to

\[
\langle \vec{r} \rangle_t = \vec{r}_0 + \Delta t \vec{v}_0 \quad (7.19)
\]

with the group momentum unchanged

\[
\frac{1}{\hbar} \langle \vec{p} \rangle_t = \vec{k}_0 . \quad (7.20)
\]

It should be recognize this as the classical motion of a particle subject to no external forces. This ob-
servation is a reflection of the Ehrenfest theorem of classical correspondence [4, p242]. Notice, however, that the width also changes by

\[
\alpha_t^2 = \alpha_0^2 + \frac{i\hbar \Delta t}{m},
\]

\[
|\alpha_t^2| = \alpha_0^2 + \frac{\hbar \Delta t}{m},
\]

meaning the state becomes wider with time. For classical-sized particles and time intervals

\[
m \gg \frac{\hbar \Delta t}{\alpha_0^2},
\]

meaning that \(\alpha_t^2 \approx \alpha_0^2\) for all practical purposes. This increase in width is thus a purely quantum mechanical phenomenon. The reader is referred to [49, p33-35][4, p64-66] for a detailed discussion, where it is explained that this is the result of the time-energy uncertainty constraint of quantum mechanics. It is also important to point out that the state gets wider independent of how fast it is traveling, and is simply a function of mass and the time interval for free propagation.

To extend the usefulness of the FEP to the arbitrary case, an alternative approach needs to be adopted. Start by writing the initial state in terms of the Dirac delta function [2], which is

\[
\psi(\vec{r}'; t_0) = \int_{\mathbb{R}^D} d\vec{r}'' \delta(\vec{r}'' - \vec{r}') \psi(\vec{r}''; t_0),
\]

where it should be noted that the only \(\vec{r}''\) dependence under the integrand is in the delta function. Now applying the FEP to this expression,

\[
\rho_f(\nabla^2_{\vec{r}'}; \Delta t) \psi(\vec{r}'; t_0) = \rho_f(\nabla^2_{\vec{r}'}; \Delta t) \int_{\mathbb{R}^D} d\vec{r}'' \delta(\vec{r}'' - \vec{r}) \psi(\vec{r}''; t_0)
\]

and noting that the propagator acts only on the \(\vec{r}''\) variables, yields

\[
\rho_f(\nabla^2_{\vec{r}'}; \Delta t) \psi(\vec{r}'; t_0) = \int_{\mathbb{R}^D} d\vec{r}'' \left[ \rho_f(\nabla^2_{\vec{r}'}; \Delta t) \delta(\vec{r}'' - \vec{r})\right] \psi(\vec{r}''; t_0).
\]

(7.25)
The quantity in the brackets \([- \cdots \] \) can be evaluated by expanding the delta functional in terms of plane waves

\[
\delta(\vec{r}'' - \vec{r}') = \langle \vec{r}' | \vec{r}'' \rangle \quad (7.26a)
\]

\[
= \langle \vec{r}' \rangle \left( \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \langle \vec{k}' \rangle \langle \vec{k}' | \vec{r}'' \rangle \right) \quad (7.26b)
\]

\[
= \langle \vec{r}' \rangle \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \langle \vec{k}' \rangle \langle \vec{k}' | \vec{r}'' \rangle \quad (7.26c)
\]

and then applying the propagator

\[
\rho_f(\nabla^2_r; \Delta t) \delta(\vec{r}'' - \vec{r}') = \langle \vec{r}' \rangle \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \left[ \exp \left( -\frac{\hbar^2 \Delta t}{2m^2} - \hbar^2 \nabla^2_r \right) \right] \langle \vec{r}' \rangle \langle \vec{k}' \rangle \langle \vec{k}' | \vec{r}'' \rangle \quad (7.27a)
\]

\[
= \langle \vec{r}' \rangle \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \left[ \exp \left( -\frac{\hbar \Delta t}{2m} \cdot \vec{k} \cdot \vec{k} \right) \right] \langle \vec{r}' \rangle \langle \vec{k}' \rangle \langle \vec{k}' | \vec{r}'' \rangle \quad (7.27b)
\]

\[
= \left( \frac{1}{2\pi} \right)^D \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \exp \left( \frac{\hbar \Delta t}{2m} \cdot \vec{k}' - \frac{\hbar \Delta t}{2m} \cdot \vec{k} \cdot \vec{k} \right) \quad (7.27c)
\]

Evaluating the integral [157, p98] results in

\[
= \left( \frac{1}{2\pi} \right)^D \hbar^D \int_{\mathbb{R}^D} d\vec{k}' \exp \left( \frac{\hbar \Delta t}{2m} \cdot \vec{k}' - \frac{\hbar \Delta t}{2m} \cdot \vec{k} \cdot \vec{k} \right) \quad (7.28)
\]

\[
= \left( \frac{1}{2\pi} \right)^D \exp \left( -\frac{1}{2} \frac{m}{\hbar^2 \Delta t} \left( \vec{r} - \vec{r}'' \right)^2 \right) \quad (7.28)
\]

The expression\(^2\)

\[
G_f(\vec{r} - \vec{r}'; \Delta t) = \left( \frac{1}{2\pi \hbar^2 \Delta t} \right)^{D/2} \exp \left( -\frac{1}{2} \frac{m}{\hbar^2 \Delta t} \left( \vec{r} - \vec{r}' \right)^2 \right) \quad (7.29)
\]

where

\[
\beta^2_t = \frac{\hbar^2 \Delta t}{m} \quad (7.30)
\]

is the integral kernel or Green function form of the FEP [144]. The effect of the FEP thus can be

\(^2\)note that \((\vec{r} - \vec{r}')^2 = (\vec{r}' - \vec{r})^2\)
formulated as

$$\psi(\vec{r}'; t_0 + \Delta t) = \int_{\mathbb{R}^D} d\vec{r}'' G_f(\vec{r}'' - \vec{r}'; \Delta t) \psi(\vec{r}''; t_0)$$  \hspace{1cm} (7.31)$$

$$\psi(\vec{r}'; t_0 + \Delta t) = \left(\frac{1}{2\pi m \Delta t}\right)^{D/2} \int_{\mathbb{R}^D} d\vec{r}'' \exp\left(-\frac{m}{2\Delta t} (\vec{r}'' - \vec{r})^2\right) \psi(\vec{r}''; t_0).$$  \hspace{1cm} (7.32)$$

It is instructive to examine a few properties of the Greens function form of the FEP. First it should be obvious that as the time-step approaches zero,

$$\lim_{\Delta t \to 0} G_f(\vec{r}' - \vec{r}; \Delta t) = \delta(\vec{r}' - \vec{r}) ,$$  \hspace{1cm} (7.33)$$

the propagator converges to the delta Functional [130, p111]. The modulus of the propagator,

$$|G_f(\vec{r} - \vec{r}'; \Delta t)| = \sqrt{G_f^* G_f} ,$$  \hspace{1cm} (7.34)$$

is constant (i.e. no dependence on position), and is equal to

$$\left(\frac{1}{2\pi m} \right)^{D/2} = \left(\frac{\pi}{2m \Delta t}\right)^{D/2} .$$  \hspace{1cm} (7.35)$$

The consequence of this is that the propagator is completely delocalized in position.

As an example as to what these quantities look like, the $D = 2$ case is plotted in figure 7.2 (see appendix 7A). It should be noted the real and imaginary parts of the propagator are only depend on the distance $|\vec{r}' - \vec{r}|$. It is also important to note that as $|\vec{r}' - \vec{r}|$ increases the real and imaginary parts become increasingly oscillatory.

The FEP in Green function form is not without its share of difficulties. Being completely delocalized and highly oscillatory makes evaluating the integral in equation 7.32 a significant challenge for both analytic and numerical treatments. Another difficulty can be seen when the time-step is taken to be
very small but not infinitesimal. The propagator expression for this situation is

\[
\left( -\frac{m}{2\pi\hbar\Delta t} \right)^{D/2} \exp \left( \frac{1}{2\hbar\Delta t} (\vec{r}' - \vec{r})^2 \right).
\]

A very large \( a \) very oscillatory function

A complex number

Such a situation is obviously a recipe for numerical disaster. It should be mentioned that there are various numerical work-arounds for avoiding these problems [132][145]-[156].

### 7.2 NCDAF Free Evolution Propagator

In the previous section, the Green function of the exact FEP was found by examining the effect of the propagator in its differential form on the delta functional. Now consider using the NCDAF approximation kernel instead of the exact delta functional. Start from the NCDAF approximation expression [see chapter 4],

\[
\tilde{\psi}(\vec{r}; M, \sigma, t_0) = \int_{\mathbb{R}^D} d\vec{r}' \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) \psi(\vec{r}'; t_0),
\]

and apply the FEP to it,

\[
\rho_f(\nabla^2_{\vec{r}}; \Delta t) \tilde{\psi}(\vec{r}; M, \sigma, t_0) = \rho_f(\nabla^2_{\vec{r}}; \Delta t) \int_{\mathbb{R}^D} d\vec{r}' \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) \psi(\vec{r}'; t_0).
\]

Since the propagator only acts on \( \vec{r} \) and the only \( \vec{r}' \) dependence under the integrand is in the NCDAF kernel, the expression can be written as

\[
\tilde{\psi}(\vec{r}; M, \sigma, t_0 + \Delta t) = \int_{\mathbb{R}^D} d\vec{r}' \left[ \rho_f(\nabla^2_{\vec{r}}; \Delta t) \tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) \right] \psi(\vec{r}'; t_0).
\]

It is useful now to recall the details of the NCDAF kernel, which are

\[
\tilde{\delta}(\vec{r}' - \vec{r}; M, \sigma) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sum_{n=0}^{M} \frac{(-1)^n}{n!} \frac{1}{(2\sigma^2)^n} \nabla_{\vec{r}'}^{2n} \exp \left( -\frac{1}{2\sigma^2} \nabla_{\vec{r}'}^2 \right).
\]
with \( \overrightarrow{R} = \overrightarrow{r}' - \overrightarrow{r} \) and \( \sigma \) is the width parameter. The effect of the propagator is thus

\[
\rho_f(\nabla^2_{\overrightarrow{r}}; \Delta t) \delta(\overrightarrow{r}' - \overrightarrow{r}; M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \sum_{n=0}^{\infty} \left( -\frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \exp \left( \frac{\hbar \Delta t}{2m} \nabla^2_{\overrightarrow{r}} \right) \left[ \nabla^2_{\overrightarrow{r}'}, \exp \left( -\frac{1}{2\sigma^2 R^2} \right) \right],
\]

and since the Laplacian in \( \overrightarrow{r}' \) commutes with the Laplacian in \( \overrightarrow{r}, \)

\[
= \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \sum_{n=0}^{\infty} \left( -\frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \nabla^2_{\overrightarrow{r}'} \left[ \exp \left( \frac{\hbar \Delta t}{2m} \nabla^2_{\overrightarrow{r}} \right) \exp \left( -\frac{1}{2\sigma^2 R^2} \right) \right].
\]

Now it is useful to notice that the generator function of the NCDAF,

\[
g(\overrightarrow{r}' - \overrightarrow{r}; \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \exp \left( -\frac{1}{2\sigma^2 (\overrightarrow{r}' - \overrightarrow{r})^2} \right),
\]

is in the form of a Gaussian Wavepacket given by equation 7.13 with \( \overrightarrow{r}_0 \Rightarrow \overrightarrow{r}, \overrightarrow{r}' \Rightarrow \overrightarrow{r}' \), \( k_0 \Rightarrow 0 \), \( \alpha \Rightarrow \sigma \), and with normalization convention adopted in chapter 2 (eq. 2.81, p 29). The effect of the FEP on such a state is given by equation 7.18, and in this case is

\[
\rho_f(\nabla^2_{\overrightarrow{r}}; \Delta t) g(\overrightarrow{r}'; \overrightarrow{r}, M, \sigma) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \rho_f(\nabla^2_{\overrightarrow{r}}; \Delta t) \exp \left( -\frac{1}{2\sigma^2 (\overrightarrow{r}' - \overrightarrow{r})^2} \right) (7.44a)
\]

\[
= \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \left( \frac{\sigma_0^2}{\sigma_t^2} \right)^{D/2} \exp \left( -\frac{1}{2\sigma_t^2 (\overrightarrow{r}' - \overrightarrow{r})^2} \right), (7.44b)
\]

where

\[
\sigma_t^2 = \sigma_0^2 + \frac{\hbar \Delta t}{m}.
\]

The result is the generator function of the NCDAF with a complex width parameter,

\[
\gamma(\overrightarrow{r}'; \overrightarrow{r}; \sigma_t) = \left( \frac{\sigma_0^2}{\sigma_t^2} \right)^{D/2} \exp \left( -\frac{1}{2\sigma_t^2 (\overrightarrow{r}' - \overrightarrow{r})^2} \right),
\]

where

\[
\sigma_t^2 = \sigma_0^2 + \frac{\hbar \Delta t}{m}. (7.46)
\]
where
\[
|\sigma_t^2| = \sigma_0^2 + \frac{\hbar^2(\Delta t)^2}{m^2}.
\] (7.47)

Using the new generator function, the expression for the NCDAF representation of the FEP can be determined. Start from the generator expression,
\[
\tilde{G}_f(\vec{r}' - \vec{r}; M, \sigma, \Delta t) = \sum_{n=0}^{M} \left( -\frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \nabla_{\vec{r}'}^{2n} \gamma(\vec{r}'; \vec{r}, \sigma_t) \quad (7.48a)
\]
\[
= \left( \frac{(\sigma_t^2)^*}{2\pi |\sigma_t^2|^2} \right)^{D/2} \sum_{n=0}^{M} \left( -\frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \nabla_{\vec{r}'}^{2n} \exp \left( -\frac{1}{2\sigma_t^2} (\vec{r}' - \vec{r})^2 \right),
\] (7.48b)

and make the variable substitutions
\[
\tilde{Z}_t = \frac{1}{\sqrt{2\pi}} (\vec{r}' - \vec{r}),
\]
\[
Z_t^2 = \frac{(\sigma_t^2)^*}{2|\sigma_t^2|^2} (\vec{r}' - \vec{r}) \cdot (\vec{r}' - \vec{r})
\] (7.49)

and
\[
(2\sigma^2)^n \nabla_{\vec{r}'}^{2n} = \left( \frac{\sigma_0^2}{\sigma_t^2} \right)^n \nabla_{\tilde{Z}_t}^{2n} \quad (7.50a)
\]
\[
= \left( \frac{\sigma_0^2}{|\sigma_t^2|^2} \right)^n \nabla_{\tilde{Z}_t}^{2n} \tilde{Z}_t
\] (7.50b)
\[
= \left( \frac{\sigma_0^2}{\sigma_0^2 + \frac{\hbar^2(\Delta t)^2}{m^2}} \right)^n \nabla_{\tilde{Z}_t}^{2n} \tilde{Z}_t
\] (7.50c)
\[
= J_t^2 \nabla_{\tilde{Z}_t}^{2n} \tilde{Z}_t,
\] (7.50d)

where
\[
J_t = \frac{1 - \frac{1}{2}\Delta t/m\sigma_0^2}{1 + \frac{\hbar^2(\Delta t)^2}{m^2\sigma_0^2}}.
\] (7.51)
The resulting expression for the NCDAF FEP in terms of the generator is

$$
\tilde{G}_f(\vec{r}' - \vec{r}; M, \sigma, \Delta \tau) = \left( \frac{\alpha_0^{1 - \text{th} \Delta \tau/m}}{2\pi(\alpha_0^{1 - \text{th} \Delta \tau/m})^2} \right)^{D/2} \sum_{n=0}^{M} \left( -\frac{1}{4} \right)^n \frac{1}{n!} J_n^2 \nabla^2_n \exp(-Z^2_\tau). 
$$  \hfill (7.52)

As with the NCDAF approximation, it is advantageous to find a polynomial expression for the NCDAF FEP. The corresponding polynomials can be found from

$$
\Lambda_n(Z^2_\tau) \exp(-Z^2_\tau) = \left( -\frac{1}{4} \right)^n \frac{1}{n!} J_n^2 \nabla^2_n \exp(-Z^2_\tau) \tag{7.53}
$$

which are proportional to the NCDAF polynomials (see chapter 3)

$$
\Lambda_n(Z^2_\tau) = J_n^2 L_n^{(D/2-1)}(Z^2_\tau) \tag{7.54}
$$

with \(\alpha = D/2 - 1\) and \(x = Z^2_\tau\). Their recursion relationship is

$$
(n + 1) \Lambda_{n+1}(Z^2_\tau) = J_n (2n - Z^2_\tau + \frac{\alpha}{2}) \Lambda_n(Z^2_\tau) - J_n^2 (n + \frac{\alpha}{2} - 1) \Lambda_{n-2}(Z^2_\tau), \tag{7.55}
$$

with the startup terms

$$
\Lambda_0(Z^2_\tau) = 1, \quad \Lambda_1(Z^2_\tau) = -J_1 \left[ Z^2_\tau - \frac{\alpha}{2} \right] \tag{7.56}
$$

The NCDAF FEP in terms of these polynomials is

$$
\tilde{G}_f(\vec{r}' - \vec{r}; M, \sigma, \Delta \tau) = \left( \frac{\alpha_0^{1 - \text{th} \Delta \tau/m}}{2\pi(\alpha_0^{1 - \text{th} \Delta \tau/m})^2} \right)^{D/2} \sum_{n=0}^{M} \Lambda_n(Z^2_\tau) \exp(-Z^2_\tau). \tag{7.57}
$$

The corresponding NCDAF approximation to the effect of the FEP is thus

$$
\tilde{\psi}(\vec{r}'; t_0 + \Delta \tau) = \left( \frac{\alpha_0^{1 - \text{th} \Delta \tau/m}}{2\pi(\alpha_0^{1 - \text{th} \Delta \tau/m})^2} \right)^{D/2} \int_{R^n} d\vec{r}' \sum_{n=0}^{M} \Lambda_n(Z^2_\tau) \exp(-Z^2_\tau) \psi(\vec{r}'; t_0). \tag{7.58}
$$
It is useful now to discuss some of the properties of the NCDAF representation of the FEP. From figure 7.3 it can be seen that the NCDAF is similar to the exact propagator in a sizable region around the origin and then smoothly decreases to zero. From figure 7.4, it can be seen that qualitatively the modulus in the position domain of the NCDAF FEP is similar to the NCDAF window [see chapter 2] in the momentum domain. Although the analytic expression for an arbitrary \( M \) is currently not known, the special case of \( M = 0 \) can easily be worked out as an example. The modulus in that case can be found,

\[
|\hat{G}_f(M = 0)|^2 = \left( \frac{\sqrt{(\sigma_0^2 + i\hbar \Delta t/m)(\sigma_0^2 - i\hbar \Delta t/m)}}{2\pi (\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2)} \right)^D \times \exp \left( -\frac{\left(\frac{\sigma_0^2}{\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2}\right)^2}{2\left(\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2\right)^2} \right),
\]

\[ (7.59a) \]

\[
= \left( \frac{\sqrt{\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2}}{2\pi (\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2)} \right)^D \exp \left( -\frac{2\sigma_0^2}{2\left(\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2\right)} \right),
\]

\[ (7.59b) \]

to be

\[
|\hat{G}_f(M = 0)| = \left( \frac{1}{2\pi (\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2)^{1/2}} \right)^{D/2} \exp \left( -\frac{\sigma_0^2}{2\left(\sigma_0^2 + \hbar^2 (\Delta t)^2/m^2\right)} \right),
\]

\[ (7.60) \]

which is a Gaussian. The important consequences are that 1) the approximate propagator is localized and 2) the problematic distant highly oscillatory contributions are now negligible. Both conditions are advantageous for using quadrature to approximate the integral in equation 7.58. The limit of the time-step approaching zero is trivially obtained by setting \( \Delta t = 0 \). The result is

\[
\lim_{\Delta t \to 0} \hat{G}_f(\vec{r}' - \vec{r}; M, \sigma, \Delta t) = \left( \frac{1}{2\pi \sigma^2} \right)^{D/2} \sum_{n=0}^{M} \frac{(-1)^n}{n!} \nabla_{\vec{r}}^{2n} \exp (-Z^2),
\]

\[ (7.61) \]
\[
\lim_{\Delta t \to 0} \tilde{G}_f(\bar{r}'; \bar{r}; M, \Delta t) = \delta(\bar{r}'; \bar{r}; M, \sigma)
\]  
(7.62)

where

\[
\begin{align*}
\lim_{\Delta t \to 0} \sigma_i^2 &= \sigma^2 \tag{7.63a} \\
\lim_{\Delta t \to 0} \bar{Z}_t &= \bar{Z} = \frac{1}{\sqrt{2\sigma}} (\bar{r}' - \bar{r}) \tag{7.63b}
\end{align*}
\]

have been used. As long as \( \sigma_0 \) is not a very small number, the near \( \Delta t = 0 \) limit avoids all the problems of the exact case.

As a side note, the modulus of the DAF illustrates another difference between the NCDAF and CPDAF approaches [chapter 5]. This is pictorially demonstrated in figure 7.4, where the CPDAF FEP clearly has a square shape whereas the NCDAF FEP is spherically symmetric.

### 7.3 Discretization and Numerical Concerns

For an arbitrary initial state the common approach is to evaluate the integral of equation 7.58 by quadrature on a grid; that is, the integral is approximated by a summation, symbolized by

\[
\int_{R^d} d\bar{r}' \approx \sum_i \Delta_i'
\]

(7.64)

where \( \Delta_i' \) is the quadrature weight for the \( i^{th} \) sampled point. Since the NCDAF FEP kernel is localized the summation can be taken over the finite number of points using some sort of cut-off criteria, such as

\[
\left\{ i \left| |\tilde{G}_f(\frac{1}{2\Delta t} (\bar{r}_i' - \bar{r}); M, \sigma, \Delta t)| < \varepsilon \right. \right\},
\]

(7.65)

where \( \varepsilon \) is a conveniently small number. The discretized version of the NCDAF FEP approximation is
thus

\[ \tilde{\psi}(\vec{r}; t_0 + \Delta t) \approx \left( \frac{\sigma_k^2 - \frac{1}{2} \Delta t / m}{2\pi(\sigma_1^2 + \hbar^2(\Delta t)^2 / m^2)} \right)^{D/2} \sum_{i} \Delta_{\epsilon} \sum_{n=0}^{M} \Lambda_{\epsilon}^{(i)}(Z_i^2) \exp \left( - \left( Z_i^2 \right) \right) \psi(\vec{r}; t_0) \]  

(7.66)

where

\[ (Z_i^2) = \frac{(\sigma_k^2 - \frac{1}{2} \Delta t / m)}{2(\sigma_1^2 + \hbar^2(\Delta t)^2 / m^2)} (\vec{r}_i^2 - \vec{r}^2) \]  

(7.67)

The choice of spatial discretization is largely dictated by the same concerns as function approximation. The sampling needs to be fine enough to make 7.64 valid. As discussed in chapter 4, the required sampling is about three times finer than what the Nyquist sampling theorem suggests. The choice of sampling spacing, however, complicated by the likelihood that a potential (in a split operator) will introduce higher frequency oscillations into the wavefunction.

There are, as of now, no rigorous rules for choosing the optimal NCDAF parameters, but a number of observational suggestions are given in reference [120]. Starting from the desired time-step ($\Delta t$) the optimal NCDAF width parameter is should be no less than

\[ \sigma \geq \sqrt{\frac{\hbar \Delta t}{m}} . \]  

(7.68)

Additionally the NCDAF width parameter $\sigma$ must be wide enough to overlap significant portions of the initial and propagated states. Counter to these concerns is a practical limitation on NCDAF width and time-step. Relatively large widths ($\sigma_x$) associated with large time-steps result in very large effective NCDAF bandwidths (eq. 7.65). The consequence is that the number of sampled points that can not be neglected becomes impractically large. This can be especially limiting in two or higher dimensions.

In realistic applications, large time-steps are rarely employed due to restrictions imposed by the split operator approximation. Once the NCDAF width parameter ($\sigma$) has been chosen, the appropriate $M$ parameter is easily determined based on the desired level of accuracy for approximating the initial function (see [120] and appendix 4C).
Given the limitations on time-step size, it is very likely that a desired time interval is several times larger than what is practical. The obvious solution to this dilemma is to propagate step wise. For example consider the case where the desired overall time interval is 10 time units and the largest practical time-step is only 0.1 time units. It is then a simple matter of repeating the propagation 100 times to reach the end of the desired interval. This situation presents a difficulty for the NCDAF FEP. Recall from chapter 4 that, the NCDAF identity kernel is not a projection operator [section 4.5.6]. The more times the propagator is applied the worse the approximation of the function will become. Experience has shown that for a well-tempered approximation [see chapter 4] the NCDAF error can grow as fast as a linear function of the number of applications. For example, if an initial error is of the order of $10^{-13}$ then after 1000 steps the error due to the NCDAF approximation would be about $10^{-10}$. Typically one just improves the fit of the initial function so NCDAF approximation error does not become comparable to error induced by the split operator approximation over the time interval.

7.4 Numerical Demonstrations

A couple example calculations will now be presented. The first will be the propagation of a Gaussian wavepacket with zero group momentum. In this case the packet will remain centered about its initial position but will increase in width with time. In the second example, the behavior of a Gaussian wavepacket with nonzero group momentum is approximated. In this case the packet will again widen but the average position will undergo classical motion. Both cases are analytically solvable so they will provide a good test of the NCDAF FEP approximation.

7.4.1 Gaussian Wavepacket with Zero Group Momentum

Plotted in figures 7.5 and 7.6 is the first test case at the initial time. The wavepacket is of the form

$$\psi(x,y) = \left(\frac{1}{\pi \alpha_x \alpha_y}\right)^{1/2} \exp\left(-\frac{1}{2} \left(\frac{x^2}{\alpha_x^2} + \frac{y^2}{\alpha_y^2}\right)\right), \quad (7.69)$$
with \( m = 1, \alpha_x = 1 \) and \( \alpha_y = 0.5 \) being the initial widths along the \( x \) and \( y \) directions respectively, and the phase factor has been chosen such that the function is completely real-valued. It is important to note that for this wavepacket \( \langle \vec{k} \rangle = 0 \), meaning it has zero group momentum; the wavepacket, however, spreads with time according to equation 7.21. This is depicted in figure 7.5. It is interesting to note that the spread,

\[
\frac{|\alpha_x^2|}{|\alpha_0^2|} = 1 + \frac{\hbar}{\alpha_0^2 m} \Delta t, \tag{7.70}
\]

increases faster along the \( y \) direction than the \( x \) direction. This is a reflection of the uncertainty principle as the more spatial localized the wavepacket is the faster it will spread.

For this system, a practical choice of parameters is \( \Delta_x = \Delta_y = 0.1, M = 18, \frac{\pi}{\Delta} = 2.0, \) and \( \Delta t = 0.3 \). This choice of parameters gives an approximation of the initial function to within 14 decimal places. It is important to note that the corresponding effective bandwidth for the NCDAF FEP is around 170 grid points. Since this means a large number of points have to be included in the approximation, it is at the upper end of practicality. The error for this the NCDAF approximation after one time-step is plotted in figure 7.7. As expected, the error is the same order of magnitude as for the approximation of the initial function.

### 7.4.2 Gaussian Wavepacket with Nonzero Group Momentum

The second example calculation involves the wavepacket described by

\[
\psi(x, y; \alpha, k_0x, k_0y) = \left( \frac{1}{\pi \alpha^2} \right)^{1/2} \exp \left( -\frac{1}{2\alpha^2} \vec{r}^2 \right) \exp \left( i \vec{k}_0 \cdot \vec{r} \right), \tag{7.71}
\]

where \( m = 1, \alpha_x = \alpha_y = \alpha = 1, \langle k_x \rangle = 0, \) and \( \langle k_y \rangle = 5 \). This wavepacket has nonzero group momentum meaning that after \( \Delta t \) it will be of the form

\[
\psi(x, y; \alpha, k_0x, k_0y) = \left( \frac{1}{\pi \alpha^2} \right)^{1/2} \exp \left( -\frac{(\vec{r}^2 - \vec{r}_0^2 - \Delta t \vec{v}_0^2)^2}{2\alpha^2} \right) \exp \left( i \vec{k}_0 \cdot \left( \vec{r}^2 - \frac{\vec{v}_0^2}{2} \Delta t \right) \right), \tag{7.72}
\]
where $\alpha_i^2 = \alpha_i^0 + \hbar \frac{\Delta t}{m}$ and $\vec{v}_0$ is the group velocity; that is, the center of the wavepacket moves along the $y$ direction with the velocity of five velocity units. Figures 7.8 and 7.9 depicts the evolution of the wavepacket over five time-steps of $\Delta t = 0.3$. It can be seen that the center of the wavepacket moves 7.5 length units along the $y$-axis as the width spreads according to equation 7.21. Figure 7.10 shows that the real and imaginary parts of this wavepacket are considerably more oscillatory than the first example (figure 7.6).

In this trial the same set of parameters as the first example ($\Delta x = \Delta y = 0.1$, $M = 18$, $\frac{\hbar}{\Delta} = 2.0$, and $\Delta t = 0.3$) were used. The error after one step is plotted in figure 7.11 which shows an accuracy of about 14 decimal places. As with the first example, the error is essentially the same magnitude as the initial approximation. The effect on the error from repeated propagation steps is depicted in figure 7.12. It is encouraging to see that after five time-steps that the error has grown less than a half an order of magnitude.
Appendix 7A: Real and Imaginary Parts of the Free Evolution Propagator

In this appendix the expressions for the real and imaginary parts of the FEP are derived for 1, 2, and 3 dimensions. Start by rewrite equation 7.29 as

\[ \left( \frac{-1}{2\pi\hbar\Delta t} \right)^{D/2} \exp \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) = \left( \frac{-1}{2\pi\hbar\Delta t} \right)^{D/2} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + i \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right]. \]  

(7A.1)

Since the details depend on the number of dimensions, each case will be examined separately. When \( D = 1 \), the expression

\[ \sqrt{-1} \left\{ \frac{m}{2\pi\hbar\Delta t} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + i \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right] \right\}, \]  

(7A.2)

can be separated by using \( \sqrt{\pm 1} = \frac{1}{\sqrt{2}} \left[ 1 \pm i \right] \) to give

\[ = \frac{1}{\sqrt{2}} \left[ 1 - i \right] \left\{ \frac{m}{2\pi\hbar\Delta t} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + i \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right] \right\}, \]  

(7A.3a)

\[ = \sqrt{\frac{1}{2}} \left\{ \frac{m}{2\pi\hbar\Delta t} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + i \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right] \right\} - \sqrt{\frac{1}{2}} \left\{ \frac{m}{2\pi\hbar\Delta t} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + i \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right] \right\}. \]  

(7A.3b)

The real and imaginary parts of the FEP for the \( D = 1 \) case are thus

\[ \text{Re}(G_f) = \sqrt{\frac{1}{2}} \left( \frac{m}{2\pi\hbar\Delta t} \right)^{1/2} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) + \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right], \]  

(7A.4)

\[ \text{Im}(G_f) = -\sqrt{\frac{1}{2}} \left( \frac{m}{2\pi\hbar\Delta t} \right)^{1/2} \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) - \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right]. \]  

When \( D = 2 \), the expression

\[ - \left( \frac{m}{2\pi\hbar\Delta t} \right) \left[ \cos \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) - \sin \left( \frac{m}{2\hbar\Delta t} (r'^2 - \bar{r}^2) \right) \right], \]  

(7A.5)
separates into the real and imaginary parts as

\[
\begin{align*}
\text{Re}(G_f) &= \left( \frac{m}{2\pi \hbar \Delta t} \right) \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right), \\
\text{Im}(G_f) &= - \left( \frac{m}{2\pi \hbar \Delta t} \right) \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right).
\end{align*}
\]  

(7A.6)

When \( D = 3 \), the expression

\[
\sqrt{-1} \sqrt{\frac{m}{2\pi \hbar \Delta t}} \left( -1 \frac{m}{2\pi h \Delta t} \right) \left[ \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) + \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right],
\]  

(7A.7)

separates by

\[
\begin{align*}
= & \left( \frac{1}{\sqrt{2}} \right) \left[ 1 - 1 \left( \frac{m}{2\pi \hbar \Delta t} \right)^{3/2} \left[ -1 \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) + \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right] \right] \quad (7A.8a) \\
= & \left( \frac{1}{\sqrt{2}} \right) \left( \frac{m}{2\pi \hbar \Delta t} \right)^{3/2} \left[ -1 \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) + \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right] \\
+ & \left( \frac{1}{\sqrt{2}} \right) \left( \frac{m}{2\pi \hbar \Delta t} \right)^{3/2} \left[ - \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) - \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right] ,
\end{align*}
\]  

yielding the real and imaginary parts as

\[
\begin{align*}
\text{Re}(G_f) &= \sqrt{\frac{1}{2}} \left( \frac{m}{2\pi \hbar \Delta t} \right)^{3/2} \left[ - \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) + \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right], \\
\text{Im}(G_f) &= - \sqrt{\frac{1}{2}} \left( \frac{m}{2\pi \hbar \Delta t} \right)^{3/2} \left[ \cos \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) + \sin \left( \frac{m}{2\pi \hbar t} (\vec{r}' - \vec{r})^2 \right) \right].
\end{align*}
\]  

(7A.9)
Appendix 7B: NCDAF Diffusion Propagator

Mathematically similar to the FEP but arising from completely different physically considerations is the diffusion propagator. It is of the form

$$\rho_d(\nabla^2_{\overrightarrow{r}}; \Delta t) = \exp \left( c \Delta t \nabla^2_{\overrightarrow{r}} \right),$$  \hspace{1cm} (7B.1)

which is a solution to the classical diffusion or heat equation \cite{136}

$$\frac{\partial \psi(\overrightarrow{r}; t)}{\partial t} = c \nabla^2_{\overrightarrow{r}} \psi(\overrightarrow{r}; t),$$  \hspace{1cm} (7B.2)

where $\psi$ is a distribution (e.g. temperature), $t$ is time, $\overrightarrow{r}$ are the spatial coordinates, and $c$ is the (real valued and isotropic) diffusion constant. As may be suspected, the NCDAF representation of this propagator is essentially the same form as that of the FEP. Instead of writing the equations down by analogy, this opportunity will be used to illustrate an alternative approach \cite[p374-377]{159} to derive the NCDAF representation.

Start from the NCDAF approximation of the initial distribution in the Fourier domain, symbolized by

$$\tilde{\Psi}(\overrightarrow{k}; t_0) = \tilde{\Delta}(\overrightarrow{k}; M, \sigma) \Psi(\overrightarrow{k}; t_0),$$  \hspace{1cm} (7B.3)

where $\Psi(\overrightarrow{k}; t_0)$ and $\tilde{\Delta}(\overrightarrow{k}; M, \sigma)$ are the Fourier transforms of $\psi(\overrightarrow{r}; t_0)$ and $\delta(\overrightarrow{r} - \overrightarrow{r}'; M, \sigma)$ respectively. This approach takes advantage of the fact that the diffusion propagator is completely local in the Fourier domain, that is

$$P_d(k^2; \Delta t) = \exp \left( c \Delta t k^2 \right) \delta(\overrightarrow{k} - \overrightarrow{k'}).$$  \hspace{1cm} (7B.4)

---

\(^3\)the reader is refered to references [160]-[162] for an alternative opinion.
The application of the propagator is thus

\[ P_d(k^2; \Delta t) \Delta(k; M, \sigma) = \exp(-cA\Delta k^2) \sum_{n=0}^{M} \exp\left(-\frac{\sigma_0^2}{2} k^2\right) \frac{1}{n!} \left(\frac{\sigma_0^2}{2} k^2\right)^n \delta(k - k') \]  

(7B.5a)

\[ = \sum_{n=0}^{M} \exp\left(-\left(\frac{\sigma_0^2}{2} + cA\Delta t\right) k^2\right) \frac{1}{n!} \left(\frac{\sigma_0^2}{2} k^2\right)^n \delta(k - k') . \]  

(7B.5b)

Defining the (real valued) quantity

\[ \sigma_t^2 = \sigma_0^2 + 2cA\Delta t , \]  

(7B.6)

(where \( \sigma_0^2 = \sigma^2 \)) allows the equation to be simplified to

\[ P_d(k^2; \Delta t) \Delta(k; M, \sigma) = \sum_{n=0}^{M} \exp\left(-\frac{\sigma_t^2}{2} k^2\right) \frac{1}{n!} \left(\frac{\sigma_t^2}{2} k^2\right)^n \]  

(7B.7a)

\[ = \exp\left(-\frac{\sigma_t^2}{2} k^2\right) \sum_{n=0}^{M} \left(\frac{\sigma_0^2}{\sigma_t^2}\right)^n \frac{1}{n!} \left(\frac{\sigma_0^2}{2} k^2\right)^n . \]  

(7B.7b)

Converting back to the position domain yields

\[ \int_{R^D} d\vec{r}' \exp\left(cA\Delta t \nabla_{\vec{r}'}^2\right) \delta(\vec{r}' - \vec{r}; M, \sigma) \psi(\vec{r}'; t_0) = \int_{R^D} d\vec{r}' \left[ \sum_{n=0}^{M} \left(-\frac{1}{4}\right)^n \frac{1}{n!} \left(\frac{\sigma_0^2}{\sigma_t^2}\right)^n \nabla_{\vec{r}'}^2 \exp\left(-Z_t^2\right) \right] \psi(\vec{r}' ; t_0) \]  

(7B.8a)

\[ = \int_{R^D} d\vec{r}' \left[ \sum_{n=0}^{M} \left(-\frac{1}{4}\right)^n \frac{1}{n!} J_t^n \nabla_{\vec{r}'}^2 \exp\left(-Z_t^2\right) \right] \psi(\vec{r}' ; t_0) , \]  

(7B.8b)

where the abbreviations \( \overrightarrow{Z_t} = (\vec{r}' - \vec{r})/\sqrt{2}\sigma_t \) and \( J_t = (\sigma_0^2/\sigma_t^2) \) have been used. This provides the generator expression form of the NCDAF Diffusion propagator

\[ \bar{G}_d(\vec{r}' - \vec{r}; \Delta t, M, \sigma_0) = \left(\frac{1}{2\pi\sigma_t^2}\right)^{D/2} \sum_{n=0}^{M} \left(-\frac{1}{4}\right)^n \frac{1}{n!} J_t^n \nabla_{\vec{r}'}^2 \exp\left(-Z_t^2\right) . \]  

(7B.9)

When compared to equation 7.52 for NCDAF FEP, the two are seen to be identical in form. The important difference is in the definition of the time dependent width \( \sigma_t \) (eq. 7.45 compared to eq.
7B.6). With this in mind all of the other expressions (eq. 7.57 to eq. 7.58) are likewise identical in form and for brevity will not be repeated.
Appendix 7C: NCDAF Representation of Metaplectic Operators

The FEP belongs to a special class of operators known as metaplectic operators [163][164]. Such operators when applied to a Gaussian function always result in another Gaussian function. One important example is the Harmonic propagator [59]. As may be suspected the Gaussian structure of the NCDAF kernel makes it particularly well suited for representing metaplectic operators.

Consider the action of a Metaplectic operator on an arbitrary state, symbolized by

\[ \phi(\vec{r}; \{a\}) = \hat{\Omega}(\vec{r}, \{\partial/\partial r\}; \{a\}) \psi(\vec{r}) , \]  

(7C.1)

where \( \vec{r}, \{\partial/\partial r\} \), and \( \{a\} \) are sets of coordinates, derivatives, and parameters respectively and \( \hat{\Omega} \) is a metaplectic operator. When the substitution of the NCDAF approximation for the actual function \( \psi \) is made, the expression becomes

\[ \hat{\Omega}(\vec{r}, \{\partial/\partial r\}; \{a\}) \tilde{\psi}(\vec{r}; \vec{M}, \sigma) = \int_{\mathbb{R}^n} \, d^2 r' \, \left[ \hat{\Omega}(\vec{r}, \{\partial/\partial r\}; \{a\}) \delta(\vec{r}' - \vec{r}; \vec{M}, \sigma) \right] \psi(\vec{r}') . \]  

(7C.2)

Now the since the metaplectic operator acts on \( \vec{r} \) it commutes with the \( \nabla_{\vec{r}}^{2n} \), of the NCDAF kernel giving

\[ \hat{\Omega} \delta(\vec{r}' - \vec{r}; \vec{M}, \sigma) \]  

(7C.3)

\[ = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sum_{n=0}^{M} \left( \frac{-1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \Omega \left[ \nabla_{\vec{r}}^{2n}, \exp\left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) \right] \]  

(7C.4)

It should be recalled that the generator function of the NCDAF,

\[ \exp(-Z^2) = \exp\left( -\frac{1}{2\sigma^2} (\vec{r}' - \vec{r})^2 \right) , \]  

(7C.5)
where \( \vec{Z} = (\vec{r}′ - \vec{r}) / \sqrt{2}\sigma \), is a Gaussian. The effect of the metaplectic operator is thus

\[
\hat{\Omega} \exp(-Z^2) = N \exp(-Z^2), \tag{7C.6}
\]

to change the generator function into a Gaussian in the new variable \( \vec{Z} \) where \( N \) is a constant factor.

In general the actual identification of this variable is a nontrivial endeavor, but for the purposes of this discussion assume it is known. The NCDAF expression for metaplectic operators in Green function form is then

\[
\hat{G}_\Omega(\vec{r}′ - \vec{r}^2; M, \sigma, \{a\}) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \int N \sum_{n=0}^{\infty} \left( -\frac{1}{4} \right)^n \frac{1}{n!} (2\sigma^2)^n \left\{ \nabla_{\vec{r}′}^n \exp(-Z^2) \right\}, \tag{7C.7}
\]

or more conveniently as

\[
\hat{G}_\Omega(\vec{r}′ - \vec{r}^2; M, \sigma, \{a\}) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \int N \sum_{n=0}^{\infty} \left( -\frac{1}{4} \right)^n \frac{1}{n!} J^n \left\{ \nabla_{\vec{r}′}^n \exp(-Z^2) \right\}, \tag{7C.8}
\]

where

\[
J = \left( \frac{\partial Z}{\partial \vec{r}′} \right)^2. \tag{7C.11}
\]

The expression

\[
\Lambda^\Omega_n(Z^2) \gamma(-Z^2) = \left( -\frac{1}{4} \right)^n \frac{1}{n!} J^n \left\{ \nabla_{\vec{r}′}^n \exp(-Z^2) \right\}, \tag{7C.12}
\]

defines a polynomial generator. It can furthermore be specified that these polynomials are proportional to the NCDAF polynomials

\[
\Lambda^\Omega_n(Z^2) = J^n \Lambda_n^{(D/2-1)}(Z^2), \tag{7C.13}
\]
in the variable $Z_i^2$. The NCDAF approximation of the effect of the metaplectic operator is thus

$$
\dot{\phi}(\vec{r}; M, \sigma, \{a\}) = \int_{\mathbb{R}^D} d\vec{r}' \hat{G}_\Omega \psi(\vec{r}')
$$

(7C.14)

$$
\dot{\phi}(\vec{r}; M, \sigma, \{a\}) = \left( \frac{1}{2\pi\sigma^2} \right)^{D/2} \sqrt{\frac{2}{\pi}} N \int_{\mathbb{R}^D} d\vec{r}' \sum_{n=0}^M \Lambda_n(Z^2) \exp(-Z^2) \psi(\vec{r}') .
$$

(7C.15)
Figure 7.1: Real part of exact FEP for $\Delta t$ (top) and $\frac{1}{2} \Delta t$ (bottom).
Figure 7.2: FEP for $D = 2$ along the diameter with $\Delta t = 0.3$, $m = 1$, and $\beta = 1$. Top: real part (solid) and modulus (dashed). Bottom: imaginary part (solid) and modulus (dashed).
Figure 7.3: Top: $D = 2$ NCDAF FEP along the diameter with $M = 18$, $\sigma = 2.0$, $\Delta t = 0.3$, $m = 1$, and $h = 1$. Bottom: difference from exact FEP. In both figures only the real part (solid) and modulus (dashed) are depicted.
Figure 7.4: Comparison of modulus of the NCDAF (left) and the CPDAF (right) FEPs for $D = 2$ with $M_{NC} = 18$, $\sigma_{NC} = 2.0$, $M_{CP} = 13$, $\sigma_{CP} = 2.0$, $\Delta t = 0.3$, $m = 1$, and $h = 1$.
Figure 7.5: Modulus squared of a wavepacket at initial and later time with $\langle x \rangle = \langle y \rangle = 0$, $\langle p_x \rangle = \langle p_y \rangle = 0$, $\alpha_x = 1$, $\alpha_y = 0.5$, $m = 1$, and $\hbar = 1$. Axis are in units of $\Delta x = \Delta y = 0.1$. 
Figure 7.6: Real and imaginary parts of a wavepacket at initial and later time with $\langle x \rangle = \langle y \rangle = 0$, $\langle p_x \rangle = \langle p_y \rangle = 0$, $\alpha_x = 1$, $\alpha_y = 0.5$, $m = 1$, and $\hbar = 1$. Note that the phase factor has been chosen so the wavepacket is completely real at $t = 0$. Axis are in units of $\Delta x = \Delta y = 0.1$. 
Figure 7.7: Real and imaginary parts of the error for the NCDAF approximation ($M = 18$, $\frac{\Delta t}{\Delta} = 2.0$, $\Delta_x = \Delta_y = 0.1$) of wavepacket ($\alpha_x = 1$, $\alpha_y = 0.5$, and $m = 1$) at $\Delta t = 0.3$. Axis are in units of $\Delta x = \Delta y = 0.1$. 
Figure 7.8: Contour of the modulus square of a Gaussian wavepacket \((\alpha_x = \alpha_y = 1, \langle p_y \rangle = 5, \text{and } m = 1)\) at various times. Axis are in units of \(\Delta x = \Delta y = 0.1\). The \(t = 0\) wavepacket is included in each plot for reference.
Figure 7.9: Continuation of figure 7.8.
Figure 7.10: Modulus, real, and imaginary parts of wavepacket at initial and later time with \((p_y) = 5, \alpha_x = \alpha_y = 1, m = 1, \text{ and } \hbar = 1\). Axis are in units of \(\Delta x = \Delta y = 0.1\). Axis are in units of \(\Delta x = \Delta y = 0.1\).
Figure 7.11: Real and imaginary parts of the error for the NCDAF approximation ($M = 18$, $\xi = 2.0$, $\Delta x = \Delta y = 0.1$) of wavepacket ($\alpha_x = \alpha_y = 1$, $p_y = 5$, and $m = 1$) at $\Delta t = 0.3$. Axis are in units of $\Delta x = \Delta y = 0.1$. 
Figure 7.12: Real and imaginary parts of the NCDAF residual ($M = 18$, $\frac{\Delta}{x} = 2.0$, $\Delta_x = \Delta_y = 0.1$) for wavepacket ($\alpha_x = \alpha_y = 1$, $(p_y) = 5$, and $m = 1$) propagation at various time-steps. Axes are in units of $\Delta x = \Delta y = 0.1$. 
8 Conclusion

The major findings of this thesis will now be enumerated. They are organized into 1) implementation, 2) generalization of one-dimensional DAF concepts, 3) general DAF concepts not previously studied, and 4) the isotropic nature of the NCDAF. For perspective, a few example avenues of future research will also be discussed.

Although the formalism of the NCDAF goes back to the early development of DAF theory [45], its computational implementation remained elusive for many years. This can be traced to a number of causes, but the major breakthrough was possible only after the NCDAF polynomials (section 3.1) and the corresponding NCμ-Wavelets (section 3.2) were characterized. Implementations of the previously derived [45][100] NCDAF function, Laplacian (sections 4.1, 4.4, and 4.5.4) and free evolution propagator (chapter 7) approximations then easily followed. Additionally, the expressions for the NCDAF gradient and Hessian were derived (section 4.1) and their implementation demonstrated (section 4.5.4).

A number of one-dimensional DAF concepts (e.g. [54][75][55][22][113][30]) have been generalized to the multi-dimensional non-Cartesian approach. The NCDAF has been shown to be related to the uncertainty principle via a constrained minimization of an appropriate uncertainty product (chapter 2). The NCDAF was also shown to share many important properties with the (unconstrained) minimum uncertainty state (section 2.4). Through scaling of the width parameter along with proper choice of polynomial degree, the NCDAF can be made arbitrarily close to the (isotropic) ideal filter (section 2.4). The ladder operators of the NCμ-Wavelets were derived using an alternative approach to the one-dimensional case (section 3.2 and 3.3). The results not only validated the previous study, they also produced a new pair of operators with more advantageous properties. The numerical foundation of the continuous (section 4.3) and the discrete (section 4.4) NCDAF approximations was also established. Many important DAF numerical properties were demonstrated to be present in the non-Cartesian generalization (section 4.5 and 4.6). They include the exact representation of polynomials (section 4.5.2 and 5.5), uniform approximation of functions and derivatives (section 4.5.5), and the well-tempered
property (section 4.6.1). The NCDAF generalization of the DAF data augmentation method was also derived and demonstrated (chapter 6).

A few general DAF concepts have been discussed. Although familiar to many researchers using DAF based methods (e.g. [121]), none has been studied in detail. The first is the DAF approximation of functions with discontinuities (section 4.5.7). The second is the discrete DAF in the momentum representation (section 4.6.2). The third is an important limitation on the accuracy of the discrete DAF (section 4.6.3 and appendix 4C).

The important consequences of the isotropic structure of the NCDAF were demonstrated (chapter 5). The uncertainty product of the NCDAF was shown to be invariant to isotropic dilations of width, but to increase with anisotropic dilations (section 2.4). The NCDAF approximation of functions was shown to be independent of the orientation of the data (section 5.6). The NCDAF approximation was also shown to be free of artificial rectangular structure that is inherent to methods based on Cartesian product structures (section 5.7).

There are numerous paths for future research stemming from this thesis. Listed below are just three representative examples in the areas of physical theory, technology, and numerical applications.

The ladder operator treatment of the NCμ-Wavelets indicated a connection to the D-dimensional (isotropic) harmonic oscillator. This relationship previously was rigorously established in the special case of one degree of freedom [55]. The difficulty in generalizing these results to the arbitrary dimensional case is that NCμ-Wavelets for angular states greater than one (i.e. \( l > 1 \)) have not been characterized. Furthermore, the ladder operators that step an arbitrary \( l \) index up and down have not been identified. An important application of the connection of NCμ-Wavelets to the D-dimensional (isotropic) harmonic oscillator is in supersymmetric quantum mechanics (SUSY-QM) theory [165]. In SUSY-QM treatment of the harmonic oscillator the even parity states correspond to bosons and the odd parity states to fermions. Preliminary work [166] for the special case of one degree of freedom suggests a completely analogous situation exists for the SUSY treatment of NCμ-Wavelets. To generalize the results to the more interesting multi-dimensional cases, characterization of all possible types of even and odd parity
NCμ-Wavelets needs to be made.

Mentioned, but not demonstrated, is adaptability of the discrete NCDAF approximation method to uniform grids other than rectangular meshes. One mesh with important applications is the hexagonal grid [111]. For example, hexagonal sampling is routinely employed in computer vision technology [167]. Preliminary results show that the discrete NCDAF sampled on a hexagonal grid can 1) provide a continuous approximation free of artifacts due to the grid, and 2) approximate linear operators, such as the Laplacian, accurately. Both properties are highly advantageous for processing collected by hexagonal sampling.

The NCDAF data augmentation method has a number of potential applications. The most obvious are image and video restoration. It is useful to mention a couple non-obvious examples. Recall that the NCDAF data augmentation method provides a poor approximation when the underlying function in the unknown gap contains a discontinuity or non-analytic feature (section 6.2.2). This can be exploited to detect local features in the data. The procedure would be based on comparing the known data in an area (or volume) with a NCDAF approximation of the data, with the actual data taken as unknown. Large errors in the approximation would be indicative of a local feature in the region under consideration. A problem where this feature detection method would be useful is in identifying cancerous tumors in mammograms. The second example of a novel application of the NCDAF data augmentation method is the extraction of scattering information from short time dynamics. The problem is that the correlation functions for scattering events that involve tunneling can take an extremely long time to decay to zero. Since each time-step involves a considerable amount of computational resources, it is advantageous to stop the calculation as early as possible. The strategy is to 1) evolve the system until the interaction is sufficiently probed, and then 2) use the NCDAF data augmentation method to extrapolate the remainder of the correlation function.
References


[47] W. Heisenberg, Physical Principles of Quantum Theory (Dover, 1930)

[48] W. Heisenberg Z. Phys. 33, p879 (1925)

[49] A. Goswami, Quantum Mechanics (Wm. C. Brown, 1992)


URL: http://physicsweb.org/articles/world/12/2/8/1


[71] Khalid Sayood, Introduction to Data Compression, 2nd Ed. (Morgan Kaufmann, 2000)


[74] Tian Xiao He (ed.), Wavelet Analysis and Multiresolution Methods (Marcel Dekker, 2001)


[77] Albert Messiah, Quantum Mechanics (Dover, 2000)

[78] H.P. Robertson, Phys. Rev. 46, p794 (1934)

[79] Leon Brillouin, Tensors in Mechanics and Elasticity (1936)


[97] L. J. Van Vliet, B. Rieger, and P. W. Verbeek, "Fourier Transform of a Gaussian" URL:

http://mathworld.wolfram.com/Hypersphere.html

http://mathworld.wolfram.com/Curvature.html

[100] David K Hoffman, unpublished (personal designation B:\0499\042399.tex, 1999)


http://mathworld.wolfram.com/LaguerrePolynomial.html


http://mathworld.wolfram.com/Hessian.html


[129] E. Merzbacher, Quantum Mechanics (Wiley, 1961)


[136] Seizo Ito, Diffusion Equations (AMS, 1992)

[137] R. Feynman, Statistical Mechanics (Benjamin, 1972)


[142] J.L. Powell and B. Crasemann, Quantum Mechanics (Addison-Wesley, 1961)


http://mathworld.wolfram.com/SquareRoot.html


[166] Yong Lee, Donald J. Kouri, David K. Hoffman, "Minimum Uncertainty Wavelets in SUSY Quantum Mechanics, the Theory of Coherent States, and String Theory" (in preparation)

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