Optimal Moment Sets for Multivariate Direct Quadrature Method of Moments

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Abstract
The direct quadrature method of moments (DQMOM) can be employed to close population balance equations (PBEs) governing a wide class of multivariate number density functions (NDFs). Such equations occur over a vast range of scientific applications, including aerosol science, kinetic theory, multiphase flows, turbulence modeling, and control theory, to name just a few. As the name implies, DQMOM uses quadrature weights and abscissas to approximate the moments of the NDF, and the number of quadrature nodes determines the accuracy of the closure. For nondegenerate univariate cases (i.e., a sufficiently smooth NDF), the N weights and N abscissas are uniquely determined by the first 2N non-negative integer moments of the NDF. Moreover, an efficient product-difference algorithm exists to compute the weights and abscissas from the moments. In contrast, for a d-dimensional NDF, a total of \((1 + d)N\) multivariate moments are required to determine the weights and abscissas, and poor choices for the moment set can lead to nonunique abscissas and even negative weights. In this work, it is demonstrated that optimal moment sets exist for multivariate DQMOM when \(N \leq nd\) quadrature nodes are employed to represent a d-dimensional NDF with \(n = 1-3\) and \(d = 1-3\). Moreover, this choice is independent of the source terms in the PBE governing the time evolution of the NDF. A multivariate Fokker-Planck equation is used to illustrate the numerical properties of the method for \(d = 3\) with \(n = 2\) and 3.

Disciplines
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Optimal Moment Sets for Multivariate Direct Quadrature Method of Moments

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The direct quadrature method of moments (DQMOM) can be employed to close population balance equations (PBEs) governing a wide class of multivariate number density functions (NDFs). Such equations occur over a vast range of scientific applications, including aerosol science, kinetic theory, multiphase flows, turbulence modeling, and control theory, to name just a few. As the name implies, DQMOM uses quadrature weights and abscissas to approximate the moments of the NDF, and the number of quadrature nodes determines the accuracy of the closure. For nondegenerate univariate cases (i.e., a sufficiently smooth NDF), the \( N \) weights and \( N \) abscissas are uniquely determined by the first \( 2N \) non-negative integer moments of the NDF. Moreover, an efficient product–difference algorithm exists to compute the weights and abscissas from the moments. In contrast, for a \( d \)-dimensional NDF, a total of \((1 + d)N\) multivariate moments are required to determine the weights and abscissas, and poor choices for the moment set can lead to nonunique abscissas and even negative weights. In this work, it is demonstrated that optimal moment sets exist for multivariate DQMOM when \( N = n^d \) quadrature nodes are employed to represent a \( d \)-dimensional NDF with \( n = 1 - 3 \) and \( d = 1 - 3 \). Moreover, this choice is independent of the source terms in the PBE governing the time evolution of the NDF. A multivariate Fokker–Planck equation is used to illustrate the numerical properties of the method for \( d = 3 \) with \( n = 2 \) and 3.

Introduction

Many problems in the physical sciences can be formulated mathematically in terms of a population balance equation (PBE) for a high-dimensional distribution function. Examples include the kinetic theory of rarefied gases,\(^1\)–\(^5\) sprays of liquid droplets,\(^6\)–\(^11\) dilute gas–solid flows,\(^12\)–\(^15\) aerosols,\(^16\)–\(^23\) colloids,\(^22\)–\(^24\) and turbulent reacting flows.\(^25\),\(^26\) In many cases, the PBEs arise in the stochastic analysis of chemically reacting systems, which has been a very active area in chemical engineering for more than 20 years.\(^27\)–\(^32\) From a computational standpoint, the treatment of many important chemical engineering problems is extremely challenging, because of the high dimensionality of the PBE (i.e., the number of degrees of freedom in the distribution function, space, and time.) In all but the simplest problems, a direct discretization of the PBE will be intractable and alternative computational strategies must be employed. Of these, the two most widely used are (1) moment methods\(^4\) and (2) Monte Carlo simulations.\(^2\),\(^8\) In addition, hybrid methods have also been developed to reduce the number of degrees of freedoms by introducing conditional moments,\(^7\),\(^10\) or to reduce statistical fluctuations by solving moment equations coupled to Monte Carlo simulations.\(^26\)

For most problems of scientific and engineering interest, the moment equations found from the PBE will not be closed. Thus, while computationally very attractive, because of their relatively low cost, the accuracy of moment methods will be determined by the accuracy of the model used to close the moment equations. A classical example is the kinetic theory of gases where accurate moment closures and numerical schemes exist for very small Knudsen numbers,\(^3\)–\(^5\),\(^33\)–\(^35\) but treatment of Knudsen numbers of order one requires direct solution of the kinetic equation\(^3\) or Monte Carlo simulations.\(^3\) Therefore, it is of continuing interest to develop accurate moment methods by considering improved closure strategies. One such strategy is the quadrature method of moments (Q MOM), which was introduced by McGraw\(^19\) and has since been used by many others.\(^6,12,18,20,22–24\) The mathematical foundations of QMOM for univariate distribution functions follow from the theory of canonical moments.\(^36\) The basic idea is that if \( \mu_k, k = 0, \ldots, 2N - 1 \), are the integer moments of a smooth univariate distribution function \( f(x), x \in (0, 1) \), then these moments can be expressed in terms of \( N \) quadrature weights \( w_n \geq 0 \) and \( N \) abscissas \( x_n \in (0, 1) \): \( \mu_k = \sum_n w_n x_n^k \). In other words, the quadrature weights and abscissas are nonlinear functions of the first \( 2N \) integer moments. Any other moment of \( f(x) \) is approximated using the weights and abscissas: e.g., \( \mu_{k+1/2} = \sum_n w_n x_n^{(2k+1)/2} \). From a computational standpoint, QMOM is attractive for univariate problems, because the weights and abscissas can be efficiently and accurately determined using the product–difference (PD) algorithm of Gordon.\(^37\) As with other numerical quadrature schemes (e.g., Gaussian quadrature), the accuracy of QMOM increases with \( N \),\(^19\) and, in most applications, \( N \) values in the range of 2–5 suffice.\(^18\)

In most reported applications of QMOM to spatially inhomogeneous PBEs,\(^18,21–23\) the distribution function does not involve the velocity and, therefore, the moments behave as passive scalars. However, in recent work,\(^6,12,38\) QMOM has been applied to the kinetic equation where the distribution function describes the velocity. By employing appropriate numerical schemes for hyperbolic kinetic equations,\(^5,33,39,40\) it was demonstrated\(^\text{a}\) that quadrature-based moment closures can describe highly nonequilibrium flows such as impinging particle jets and particle rebound off walls. In the context of the kinetic equation, the key property of quadrature methods that makes the description of nonequilibrium flows possible is that each node is advected with its own velocity.\(^12,38\) These node velocities are determined at each point in the flow by inverting the moment equations to determine the weights and abscissas. In one-dimensional (1D) problems, this can be done using the PD algorithm. However, in two-dimensional (2D) and three-dimensional (3D) problems, the PD algorithm no longer is applicable and other approaches are needed to invert the moment

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equations. In previous work, the inversion formulas are restricted to cases with \( N = 2 \) nodes, which limits the ability of the method to capture certain second-order moments. In subsequent work, Fox extended the inversion formulas to \( N = 8 \) nodes and third-order moments.

For multivariate PBEs, to use QMOM with \( N > 2 \), it is necessary to invert the moment equations numerically. An alternative approach is to use the direct quadrature method of moments (DQMOM) instead of the moments, to solve for the weights and abscissas directly. Questions then arise concerning what choice of moments should be used and whether the DQMOM equations are well-defined. Moreover, even if the inversion is well-defined, for some choices of \( N \) it can arise for which the weights are negative (i.e., unphysical). Because of the nonlinearity of the inversion problem, it is extremely difficult to determine in advance whether a particular choice of moments and \( N \) will lead to realizable weights and abscissas. Thus, the goal of this work is to identify moment sets for particular values of \( N \) that will lead to realizable weights and abscissas for multivariate problems. We begin by reviewing the DQMOM problem formulation and introduce the notation used in the rest of the paper. We then introduce the concept of “optimal moment sets” and show examples of such moments in two and three dimensions. Finally, an application of DQOM with the optimal moment sets to the multivariate Fokker–Planck equation is proposed, followed by conclusions. On a personal note, it is a great pleasure to dedicate this paper in honor of the many contributions to chemical engineering science made by Dr. B. D. Kulkarni, whose early work in stochastic modeling roughly corresponds to the start of my own interest in the subject.

Problem Formulation

In this work, we consider computational methods for approximating the solution to the PBE for a multivariate number density function (NDF), denoted by \( f(x) \), where \( x \) is the property vector. Such NDF occur in numerous scientific and technological applications. For example, in kinetic theory, the variables \( x \) correspond to the velocity of a particle, and \( f(x) \ dx \) is the probability of finding a particle with a given value of \( x \), whereas in aerosol science, the variable \( x \) can denote the mass, surface area, and chemical composition of droplets. (See the earlier works for example PBEs from chemical reaction engineering and multiphase flow.) Generally, a PBE of the form

\[
\frac{\partial f}{\partial t} = S(x, f)
\]

will be available, and our goal is to find solutions for \( f \) that satisfy this equation. The right-hand side (RHS) of eq 1 is application-dependent, but often it is nonlinear in \( x, f \), or both, making it impossible to derive analytical solutions. Various methods have been proposed in the literature to approximate \( f \), but it is fair to say that most of them become intractable when the dimensionality of \( x \) is \( > 2 \). For such cases, it is often necessary to revert to stochastic approximations for eq 1 that yield estimates for \( f \) based on a finite ensemble of notional particles. While stochastic methods are usually straightforward to implement for any value of \( d \), they require suitable averaging to minimize the inherent statistical noise. For example, even the low-order moments of the NDF estimated from stochastic methods can exhibit large statistical fluctuations.

As an alternative to solving for \( f \) directly, moment methods transform eq 1 to

\[
\frac{\partial m(k)}{\partial t} = S_k
\]

where the moments of the NDF are defined by

\[
m(k) = \int x_1^{k_1} \cdots x_n^{k_n} f(x) \, dx
\]

and the moment source term is

\[
S_k = \int x_1^{k_1} \cdots x_n^{k_n} S(x, f) \, dx
\]

However, the major difficulty with moment methods is that the RHS of eq 2 is almost always unclosed (i.e., it cannot be expressed in terms of the moments), even when eq 1 is closed. Therefore, it is necessary to find a closure for \( S_k \) that can be truncated at a finite set of moments: \( k \in 0, \ldots, k_{\text{max}} \). A well-known example is the Grad 13-moment approximation for the Boltzmann equation from kinetic theory.

QMOM was introduced by McGraw as an efficient, yet accurate, closure for the moment source term \( S_k \) found for the moments of a univariate NDF \( f(x) \). The principal idea is related to Gaussian quadrature, and can be expressed as

\[
\int g(x)f(x) \, dx = \sum_{a=1}^{N} w_a g(x_a)
\]

where \( g \) is an arbitrary smooth function. In QMOM, the \( N \) weights \( w_a \) and \( N \) abscissas \( x_a \) are determined by solving a system of nonlinear equations for \( k = 0, \ldots, k_{\text{max}} \) with \( k_{\text{max}} = 2N - 1 \):

\[
m(k) = \sum_{a=1}^{N} w_a x_a^k
\]

where the first \( k_{\text{max}} \) moments of the NDF are assumed to be known (i.e., they are determined by solving eq 2).

For large \( N \), eq 6 is poorly conditioned; however, it can be solved accurately using the product–difference (PD) algorithm that has been described elsewhere. For nondegenerate NDFs, it can be shown that the solution to eq 6 is unique, the weights are always non-negative, and the abscissas are realizable. [An abscissa is realizable if it lies in the interior of the support of \( f \).] Therefore, the basic computational algorithm used in QMOM consists of solving transport equations for \( m(k) (k = 0, 1, \ldots, k_{\text{max}}) \) wherein the nonlinear source terms are closed using Gaussian quadrature, as shown in eq 5. The QMOM algorithm has been shown to yield accurate results for problems involving univariate density functions, including complex integro-differential expressions arising from aggregation and breakage terms.

The extension of QMOM to multivariate PBEs is challenging because the PD algorithm cannot normally be used with more than one variable. However, it is sometimes possible to solve the multivariate version of eq 6 for a selected set of multivariate moments by employing a nonlinear equation solver. The success of such an approach will be dependent, in part, on whether the weights and abscissas are uniquely determined by the chosen set of moments. Indeed, unlike in the univariate case, there is no guarantee in the multivariate case that the weights will be non-negative and the abscissas realizable for a particular choice of moments. Alternatively, DQMOM approximates the NDF through the use of weighted delta functions in phase space:

\[
f(x; t) = \sum_{a=1}^{N} w_a(t) \prod_{\beta=1}^{d} \delta(x_{\beta} - X_{a\beta}(t))
\]

where the abscissas \( X_a \) have components \( X_{a\beta} \). In terms of the weights and abscissas, the multivariate moments are given by
\[ m(k) = \sum_{a=1}^{N} w_a \prod_{\beta=1}^{d} X_{a\beta}^{\delta_{\beta}} \]  

Instead of inverting eq 8, DQ MOM solves the transport equations directly for the weights and the abscissas: \( Y_a = w_a X_a \). Note that there are now \( N \) weights and \( dN \) abscissa components that must be determined from an independent set of \((1 + d)N\) moments. The choice of this set of moments is the primary subject of this work.

Starting from eq 2, it is easily shown that the DQ MOM transport equations (one for each of the \((1 + d)N\) moments) have the form

\[ A(k, X) \frac{\partial \[ w \]}{\partial \[ Y \]} = S_k \]  

where \( w^T = [w_1 \ldots w_N] \) and \( Y^T = [Y_1^T \ldots Y_N^T] \) are vectors of length \( N \) and \( dN \), respectively. The components of the moment source vector \( S_k \) are defined as in eq 4, using eq 7 to close the NDF. In other words, \( S_k \) will be a closed function of \( w \) and \( Y \).

In the following, we will be interested in sets of \( N \) distinct, nondegenerate abscissas \( X_a \). By definition, a set of abscissas is nondegenerate if the matrix formed using the abscissas as columns (i.e., \([X_1 \ldots X_a]\)) is full rank (i.e., rank \( d \)). In a broad sense, DQ MOM can be viewed as a generalization of Grad's moment method \(^4\) (i.e., a set of moments determines the shape of the NDF), but with the difference that, in DQ MOM, the NDF is expanded in a delta-function basis, as opposed to the Hermite polynomials used by Grad.

The DQ MOM coefficient matrix \( A \) in eq 9 is square with size \((1 + d)N\), and is defined by its components:\(^{17,25}\)

\[ a_{ij} = \begin{cases} 
(1 - k_i) \prod_{a=1}^{d} X_{pa}^{x_{ja}} & \text{for } p = j, \text{ if } 1 \leq j \leq N \\
\left( \frac{k_i}{X_{ja}} \right) \prod_{a=1}^{d} X_{pa}^{x_{ja}} & \text{for } p = j - N, \text{ if } N + 1 \leq j \leq 2N \\
\vdots & \vdots \\
\left( \frac{k_i}{X_{pa}} \right) \prod_{a=1}^{d} X_{pa}^{x_{ja}} & \text{for } p = dN, \text{ if } dN + 1 \leq j \leq (1 + d)N 
\end{cases} \]

where \( k_i = (k_{i1}, \ldots, k_{id}) \) denotes the exponents for the \( i \)th moment and \( k_i = k_{i1} + \ldots + k_{id} \). Note that \( A \) is dependent only on the abscissas \( X_a \) and not on the weights. Therefore, it does not necessarily become singular when one of the weights is null (as would be the case if we did not use the weighted abscissas to define the independent variables in DQ MOM). The reader should also note that \( A \) is equal to the Jacobian matrix of the RHS of eq 8 and would be used by a nonlinear equation solver such as the Newton–Raphson method to invert the moments to determine the weights and abscissas. Thus, we can surmise that the properties of \( A \) for particular choices of moments will be of paramount importance when using any quadrature-based moment method.

The remainder of this work is devoted to understanding the properties of \( A \) for \( 1 < d \) (i.e., multivariate cases.) For \( d = 1 \), it can easily be shown that \( A \) is full rank if and only if the abscissas are distinct. The latter will always be the case if the corresponding NDF is nondegenerate. Furthermore, for the univariate case, it is possible to choose independent noninteger moments without affecting the rank of \( A \).\(^{46}\) For multivariate cases, having distinct abscissas does not guarantee that \( A \) will be full rank for every distinct choice of moments. In fact, it can be shown that for fixed \( N \) and \( d \), certain distinct moments are linearly dependent when \( 1 \leq d \) for all possible sets of abscissas.\(^{17}\) More problematically, it can also arise that \( A \) can become singular, because of the dynamics of eq 9. In other words, the initial conditions may be such that \( A \) is nonsingular, but the dynamics generated by \( S_k \) may force the abscissas to pass into a singular region of phase space.\(^{37}\) Thus, for eq 9 to represent a viable computational approach for approximating eq 1, it is necessary to identify a moment set for which \( A \) is nonsingular for all nondegenerate points in phase space for given values of \( d \) and \( N \). This is the subject of the next section.

**Optimal Moment Sets for \( 1 < d \leq 3 \)**

Before defining an optimal moment set and describing our methodology for finding them, we first make several important observations concerning the coefficient matrix \( A \).

**Properties of \( A \).** The properties of \( A \) are as follows:

1. Each moment in a moment set is specified by a unique exponent vector \( k \), and corresponds to a row in \( A \).
2. The order of a moment (\( \gamma_i \)) is defined to be the value of \( \gamma_i = k_i \). For example, with \( d = 3 \), \( k_1 = (0, 0, 0) \) is zero order (\( \gamma_1 = 0 \)), and \( k_2 = (1, 0, 0) \) is first order (\( \gamma_2 = 1 \)). The number of distinct moments of a given order is dependent on \( d \). For example, with \( d = 3 \), the number of moments of order \( \gamma = 0, 1, \ldots, 3 \) is \( (\gamma + 1)(\gamma + 2)/2 \).
3. For \( d = 1 \), there is one distinct moment for a given order (\( \gamma = i - 1 \) for \( i = 1, \ldots, 2N \)) and, provided the abscissas are distinct, the rows of \( A \) are linearly independent.
4. Numbering the moments by increasing order (i.e., \( \gamma_1 < \gamma_2 < \ldots < \gamma_{\max} \)), it can easily be shown that the first \( 1 + d \) rows of \( A \) (i.e., the zero- and first-order moments) are always linearly independent. However, the linear independence of subsequent rows with a given order is dependent on \( d \) and \( N \). For example, if \( d = N = 2 \) it can easily be shown\(^{17}\) that only two of the three second-order moments lead to independent rows in \( A \) (regardless of the values of the distinct abscissas).
5. Defining the vector \( Z^T = [w^T \; Y^T] \), eq 8 can be written as a nonlinear system of equations of the form \( F(Z) = 0 \). The linearized form of this equation yields an iteration scheme:

\[ Z_{n+1} = Z_n - A_n^{-1} F_n \]

Thus, if \( A \) is full rank at every point in phase space, then \( A_n^{-1} \) will be well-defined and \( F(Z) = 0 \) will have, at most, one solution.
6. The components of \( A \) can be rescaled using a positive scaling factor \( X_c \):

\[ a_{ij}^* = \frac{a_{ij}}{X_c^{\delta_{ij}}} \]

such that \( a_{ij}^* \) is defined by eq 10 but with \( X_{a\beta}^* = X_{a\beta}/X_c \). The matrix \( A^* \) will have the same rank as \( A \). The scaling factor is arbitrary and can always be chosen such that \( |X_{a\beta}| \leq 1 \) for all \( \alpha \) and \( \beta \).\(^{46}\) Thus, it suffices to show that \( A \) is full rank in the phase space defined by \( N \) distinct, nondegenerate abscissas with components that satisfy \( |X_{a\beta}| \leq 1 \).

**Definition of an Optimal Moment Set.** Based on the aforementioned observations, we define an optimal moment set for a given value of \( d \) to have the following properties:

1. An optimal moment set consists of \((1 + d)N\) distinct moments. [Hence, \( A \), defined using the optimal moment set, is a square matrix.]
2. An optimal moment set will yield a full-rank matrix \( A \) for all possible sets\(^{49}\) of \( N \) distinct, nondegenerate abscissas whose components satisfy \( |X_{a\beta}| \leq 1 \) for \( 1 \leq \alpha \leq N \) and \( 1 \leq \beta \leq d \).
(3) An optimal moment set includes all linearly independent moments of a particular order $\gamma_i = 2, 3, ...$ before adding moments of higher order.

Note that this definition does not imply the existence of an optimal moment set for every value of $N$. Furthermore, optimal moment sets for $N = 1$ are trivial, so we are primarily concerned with $N \geq 2$. The final property excludes moment sets that do not control lower-order moments (usually cross moments) but use high-order moments to define $A$. For example, we have shown that, for $d = 2$, it is possible to use moments in $X_1 (m(k_1, 0))$ up to order $2N - 1$ combined with moments in $X_2 (m(0, k_2))$ up to order $N - 1$. However, this would not be an optimal moment set, because it does not include cross moments such as $m(1, 1)$ or $m(1, 2)$. Generally, neglecting cross moments leads to abscissas that lie on lower-dimensional subspaces of $d$-dimensional phase space. Although lower-dimensional supports may result from the moment source terms for particular ports may result from the moment source terms for particular applications, it would not be appropriate to choose, for the general case, a moment set to define $A$ that is restricted to generating such behavior. Therefore, we shall limit ourselves to moment sets that treat all directions in phase space equally.

Note that our definition of an optimal moment set is not concerned with the accuracy of the DQ MOM approximation of “uncontrolled” moments (i.e., moments not included in the moment set). For $d = 1$, it can be shown that certain choices of moments lead to better closure of $S_i$ than other choices. However, for $d = 1$, all sets of distinct moments are optimal, making it possible to explore many possibilities to increase the accuracy for a given $N$. In contrast, for $d \geq 2$, most moment sets are not optimal (i.e., there are regions in phase space where $A$ is rank-deficient). Looking at the problem another way, choosing noninteger moments when $d = 1$ is equivalent to a change of variable $X^* = g(X)$, where $g$ is a smooth, invertible function. In other words, using integer moments for $X^*$ will yield the same results as using noninteger moments for $X$. Therefore, the extension of this idea to $d \geq 2$ will be straightforward after we have determined an optimal moment set based on integer moments, which is the primary objective of this work.

Methodology for Finding Optimal Moment Sets. The methodology that we use for finding optimal moment sets for a given $d$ and $N$ is as follows:

1. The distinct moments of a particular order are dependent on $d$. Thus, we begin by defining all possible rows of $A$ up to a maximum order of $2N$. Note that the matrix $A$ constructed in this step will have many more rows than columns.

2. Certain rows generated in the first step will be linearly dependent for any choice of abscissas. Therefore, we generate a set of $N$ “optimal” abscissas (defined below) and, starting at the lowest order, we remove rows from $A$ one at a time if they are linearly independent. This procedure terminates when $A$ is full rank and square.

3. The moment choice found in the previous step results in $A$ being full rank for a particular choice of abscissas. For the moment choice to be optimal, it must be shown that $A$ is full rank for all choices of nondegenerate abscissas. This can be done by randomly generating abscissas and checking the condition number of $A$. If the condition number is too large, relative to machine precision, the moment set is rejected as nonoptimal.

4. The “random-abscissa” test used in the previous step can miss (at least with finite samples) certain “special” cases. For example, for some values of $N$, we have found that $A$ is rank-deficient along certain directions corresponding to simple rotations of the optimal abscissas. The practical consequence of this observation is that no single set of moments will be optimal for all possible sets of initial conditions. However, we show below that it is possible to define a matrix $L$ and abscissas $X^* = LX$ such that the optimal moment set applied to $X^*$ yields a nonsingular $A$. Note that this linear transformation corresponds to defining $A$ in terms of a linear combination of the moments of $X$. (See Appendix for more details.)

5. Simulations are run using the Fokker-Planck equation described below to determine whether the weights can become negative with the proposed moment set. If negative weights are observed, the moment set is rejected as nonoptimal.

The procedure outlined above is applied for a given value of $N \geq 2$. If it fails, then no optimal moment set can be found for that value of $N$, so the procedure must be repeated with the next larger $N$.

Conjectures on the Existence of Optimal Moment Sets. Our experience with $1 \leq d \leq 3$ has been that the aforementioned procedure always yields an optimal moment set when $N = n^d$ for $n = 1, 2, 3$. Furthermore, when $N = n^d$, we have found that it suffices to check only moments whose exponents satisfy $0 \leq k_{\alpha} \leq 2n - 1$. In fact, based on our experience, we make the following four conjectures:

1. An optimal moment set for a given $d$ can be found when $N = n^d$ with $n = 1, 2, ...$

2. When $N = n^d$, an optimal moment set exists that contains all moments up to order $2n - 1$, and the $i$th moment in the set has integer exponents that satisfy $0 \leq k_{\alpha} \leq 2n - 1$ for $1 \leq i \leq (1 + d)N$ and $1 \leq \alpha \leq d$.

3. The optimal moment set that satisfies the aforementioned two conditions is unique under a linear transformation, with respect to the optimal abscissas. [As discussed earlier for $d = 1$, uniqueness is defined with respect to the sets of moments with bounded integer exponents.]

4. A linear transformation matrix $(X^* = LX)$ exists with the property that using the optimal moment set for $X^*$ results in a nonsingular $A$ for any given set of distinct, nondegenerate abscissas $X$. (See the Appendix for the exact definition of the DQ MOM linear system after applying the linear transformation.) Note that, in practice, it is usually preferable to define the abscissas in terms of the central moments (i.e., deviations about the average), in which case the linear transformation becomes an affine transformation.

Note that the total number of moments in the optimal moment set is $(1 + d)N$, and, hence, the number of moments up to order $2n - 1$ will not be sufficient to complete the set unless $d = 1$. The additional moments come from the subset of higher-order moments with bounded exponents. The third conjecture thus states that there is only one choice of moments from this set that, when combined with the moments of order up to $2n - 1$ (which themselves must be linearly independent), yields a full-rank matrix $A$ for the optimal abscissas. For nonoptimal abscissas, it will be necessary to define a transformation matrix $L$ such that the optimal moment set can be applied to the transformed abscissas.

While we do not have a formal mathematical proof, these four conjectures are based on our success in finding optimal moment sets for $d \leq 3$ and $n \leq 3$. In practice, $n$ values greater than 4 or 5 are rarely needed for DQ MOM. Moreover, with $d = 3$ and $n = 3$, the number of abscissas is already $n^d = 27$. At some point, the number of abscissas required for DQ MOM will be too large to be competitive with stochastic methods. An alternative approach (that has yet to be explored) might be to combine DQ MOM with stochastic methods. A hybrid algorithm...
of this type would be similar to variance-reduction techniques in that DQMOM would force lower-order moments (in the optimal moment set) to be exact, while letting the stochastic method generate fluctuations in the higher-order moments. It is likely that \( n = 2 \) would suffice for a hybrid method. Thus, while the existence of optimal moment sets for \( n > 3 \) is an interesting open question, we will restrict ourselves to finding optimal moment sets and linear transformation matrices \( L \) for \( d \leq 3 \) and \( n \leq 3 \) in the remainder of this paper.

**Optimal Abscissas for \( d = 2, 3 \).** The optimal abscissas \( X^* \) used in the aforementioned procedure for \( d = 3 \) are given in Table 1 for \( N = 8 \) and Table 2 for \( N = 27 \). Only the positive abscissas are shown for \( N = 27 \). The others can be found by permutations of the sign of each component. The optimal abscissas for \( d = 2 \) can be found by eliminating the third component and the resulting nondistinct abscissas. Note that the optimal abscissas enjoy certain symmetry properties that one might expect for independent random variables. Indeed, they correspond to one solution for the quadrature nodes for an independent, joint Gaussian probability density function (JIG-PDF). In this context, these abscissas are optimal (with respect to all other possible sets of abscissas), in that they reproduce the greatest number of higher-order moments (i.e., orders greater than \( 2n - 1 \)) of the JIG-PDF. However, it is important to note that the moments of the IJG-PDF are invariant under rotation:

\[
X^* = RX \leftrightarrow m^* = m(k) \leftrightarrow m(k_0) = m(k_0)
\]  

(13)

(where \( R \) is a rotation matrix), whereas the moments of order higher than \( 2n - 1 \) determined from DQMOM will not be rotationally invariant. [More generally, this property can be extended to linear transformations, as discussed in the Appendix.]

As illustrated using the optimal abscissa (111) in Figure 1, rotation of the abscissas away from the optimal values leads to singularities in \( A \). These singularities occur along curves on the surface of the sphere generated by all arbitrary rotations. Although there is a relatively large region near the optimal abscissa (111) where \( A \) is nonsingular, the presence of the singular curves will make it impossible to start at an arbitrary point on the surface of the sphere and to relax to the optimal abscissa without crossing a singular curve. To overcome this difficulty, we will use a nonsingular linear transformation \( X^* = LX \), defined such that the transformed abscissas lie "close" to the optimal abscissas \( X^* \). It will then be possible to use the optimal moment sets found using the optimal abscissas to specify the moments of \( X^* \) used to define \( A \).

In the Appendix, we show that a linear transformation of \( X \) transforms the moments such that a particular moment of \( X^* \) is a linear combinations of the moments of \( X \) of the same order. This implies that, if the optimal moment set contains all moments of \( X^* \) of a given order (e.g., orders \( 0, \ldots, 2n - 1 \)), then all moments of \( X \) of the same order will appear in the optimal moment set. In other words, all moments of order \( 2n - 1 \) and smaller will be controlled, regardless of the choice of \( L \). On the other hand, we will see below that the optimal moment set does not contain all moments of a given order for orders greater than \( 2n - 1 \). However, after the linear transformation, a given moment of \( X^* \) will usually contain a linear combination of all moments of \( X \) with the same order. Thus, the optimal moment set will control not individual moments of \( X \), but rather linear combinations of such moments. From a practical standpoint, we must therefore specify a linear-translation matrix \( L \) for each set of distinct, nondegenerate abscissas such that \( A \) is nonsingular when defined by the optimal moment set for \( X^* \).

**Optimal Moment Sets for \( d = 2 \).** For \( d = 2 \) and \( n = 2 \), there are \( N = 4 \) optimal abscissas and a total of 12 moments in the optimal set. The moment exponents are \( k_{21} \) and \( k_{22} \), and they take on integer values in the set \( \{0, 1, 2, 3\} \). The first 10 moments in the optimal moment set are the distinct moments of order three and smaller. The remaining 2 moments are \( m(3, 1) \) and \( m(1, 3) \) (order four). The complete set of optimal moments is given in Table 3.

For \( d = 2 \) and \( n = 3 \), there are \( N = 9 \) optimal abscissas and a total of 27 moments in the optimal set. The moment exponents \( k_{31} \) and \( k_{32} \) take on integer values in the set \( \{0, 1, 2, 3, 4, 5\} \). The first 21 moments in the optimal moment set are the distinct moments of order five and smaller. The remaining 6 moments are order six or seven. The complete set of optimal moments is given in Table 4.

**Optimal Moment Sets for \( d = 3 \).** For \( d = 3 \) and \( n = 2 \), there are \( N = 8 \) optimal abscissas (Table 1) and a total of 32 moments in the optimal set. The moment exponents are \( k_{31}, k_{32}, \ldots, k_{38} \).
that such a transformation exists in general, we note that when
choices of the weights and abscissas. Although no proof exists
for all possible sets of nondegenerate abscissas.

\[ \langle X^i \rangle = \sum w_i X_i, \quad \text{and a matrix } B \text{ formed from the weights}
\]

\[ B^* = [w_i(X_i^1 - \langle X^1 \rangle) \ldots w_i(X_i^d - \langle X^d \rangle)] \quad (14) \]

where \( \langle X^i \rangle = \sum w_i X_i \), and a matrix \( B \) formed from the weights
and abscissas:

\[ B = [w_i(X_i - \langle X \rangle) \ldots w_i(X_i - \langle X \rangle)] \quad (15) \]

where \( \langle X \rangle = \sum w_i X_i \). The linear-transformation matrix is then defined by\(^{57}\)

\[ L = \beta B^* (B B^*)^{-1} \quad (16) \]

and \( k_{i3} \), and they take on integer values in the set \{0, 1, 2, 3\}. The first 20 moments in the optimal moment set are the distinct
moments of order three and smaller. The remaining 12 moments
are order four or five. The complete set of optimal moments is
given in Table 5. Comparing Table 3 to Table 5, we observe
that the former can be found from the latter by eliminating
moments where \( k_3 \neq 0 \). The extension to \( d > 3 \) should follow
the same pattern. Also note that the higher-order moments
appear in symmetric combinations. For example, because
that is dependent on \( L \). This definition is equal to the rotation matrix \( R \) needed
to rotate all abscissas to the optimal abscissas, and thus \( A \) will
always be full rank for such cases.

Although it follows our intuition and works well for the
Fokker–Planck equation as shown below, no proof is available
yet to show that eq 16 will suffice for other systems. However,
because the linear transformation forms linear combinations of
all moments up to the highest order in the optimal set, it should
suffice to demonstrate that the matrix \( A \) formed using all
moments up to the highest order is always full rank. For
example, for \( n = 3 \) and \( d = 3 \), it should suffice to go up to
order nine (see Table 6). Finally, we note that, because the
definition of the linear transformation uses a rotation about the
average, it is likely that the use of central moments will improve
the performance of the algorithm. The central moments are
related to \( m(k) \) by a change of variables, and the abscissas found
from the central moments differ from \( X \) by a simple translation
by the average.\(^{58}\)

| Table 5. Optimal Moment Set for \( d = 3 \) and \( N = 8 \) |
|---|---|---|---|---|---|---|---|---|---|
| \( k_i \) | 0 | 1 | 0 | 0 | 2 | 1 | 1 | 0 | 0 |
| \( k_{i2} \) | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 2 | 1 |
| \( k_{i3} \) | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 1 |
| \( i \) | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| \( k_i \) | 3 | 2 | 2 | 1 | 1 | 1 | 0 | 0 | 0 |
| \( k_{i2} \) | 0 | 1 | 0 | 2 | 1 | 0 | 3 | 2 | 1 |
| \( k_{i3} \) | 0 | 0 | 1 | 0 | 1 | 2 | 0 | 1 | 2 |
| \( i \) | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 |
| \( k_i \) | 0 | 3 | 1 | 3 | 0 | 3 | 1 | 1 | 1 |
| \( k_{i2} \) | 1 | 0 | 0 | 3 | 1 | 3 | 1 | 1 |
| \( k_{i3} \) | 1 | 0 | 0 | 3 | 1 | 3 | 1 | 1 |

and \( k_{i3} \), and they take on integer values in the set \{0, 1, 2, 3\}. The first 20 moments in the optimal moment set are the distinct
moments of order three and smaller. The remaining 12 moments
are order four or five. The complete set of optimal moments is
given in Table 5. Comparing Table 3 to Table 5, we observe
that the former can be found from the latter by eliminating
moments where \( k_3 \neq 0 \). The extension to \( d > 3 \) should follow
the same pattern. Also note that the higher-order moments
appear in symmetric combinations. For example, because
that is dependent on \( L \). This definition is equal to the rotation matrix \( R \) needed
to rotate all abscissas to the optimal abscissas, and thus \( A \) will
always be full rank for such cases.

Although it follows our intuition and works well for the
Fokker–Planck equation as shown below, no proof is available
yet to show that eq 16 will suffice for other systems. However,
because the linear transformation forms linear combinations of
all moments up to the highest order in the optimal set, it should
suffice to demonstrate that the matrix \( A \) formed using all
moments up to the highest order is always full rank. For
example, for \( n = 3 \) and \( d = 3 \), it should suffice to go up to
order nine (see Table 6). Finally, we note that, because the
definition of the linear transformation uses a rotation about the
average, it is likely that the use of central moments will improve
the performance of the algorithm. The central moments are
related to \( m(k) \) by a change of variables, and the abscissas found
from the central moments differ from \( X \) by a simple translation
by the average.\(^{58}\)

**Application to the Fokker–Planck Equation**

In this section, we apply DQ MOM with the optimal moment
sets and the linear transformation identified in the previous
section to approximate solutions to a linear Fokker–Planck (FP)
equation. This simple closed system is investigated to facilitate
our understanding of the numerical results.

**Multivariate Fokker–Planck Equation.** The multivariate
FP equation used in this section has the form

\[ \frac{\partial f}{\partial t} = \sum_{i=1}^{d} \left( \frac{\partial}{\partial x_i} (x_i f) + \frac{\partial^2}{\partial x_i^2} f \right) \quad (17) \]

This example has been chosen because the moment source terms
can be written in closed form:

\[ S_k = -(k_1 + k_2 + k_3)m(k_1, k_2, k_3) + k_1(k_1 - 1)m(k_1 - 2, k_2, k_3) +
\]

\[ k_2(k_2 - 1)m(k_1, k_2 - 2, k_3) + k_3(k_3 - 1)m(k_1, k_2, k_3 - 2) \quad (18) \]

Thus, DQ MOM should exactly reproduce the time evolution
of all moments included in the optimal moment set\(^{58}\) (i.e., \( S_k \)
don’t require closure and the linear system given by eq 2 can
be solved directly to find \( m(k) \)). Therefore, it will be possible
to investigate numerical issues that arise from solving eq 9 and
determining \( m(k) \) from eq 8 without the additional complications
associated with closing the moment source terms.

**Steady-State Solution for FP Moments.** The FP moment
equations admit a steady-state solution of the form

\[ m_i(k_1, k_2, k_3) = m_i(k_1)m_i(k_2)m_i(k_3) \quad (19) \]

where the moments for the univariate Gaussian PDF follow the
usual recurrence relationship:
Table 7. Steady-State Weights and Optimal Abscissas for \( d = 3 \) and \( N = 8 \)

<table>
<thead>
<tr>
<th>( w )</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
<th>1/8</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_1 )</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>( X_2 )</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>( X_3 )</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 8. Steady-State Weights and (Non-Negative) Optimal Abscissas for \( d = 3 \) and \( N = 27 \)

<table>
<thead>
<tr>
<th>( w )</th>
<th>8/27</th>
<th>2/27</th>
<th>2/27</th>
<th>2/27</th>
<th>1/54</th>
<th>1/54</th>
<th>1/54</th>
<th>1/216</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_1 )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
</tr>
<tr>
<td>( X_2 )</td>
<td>0</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
</tr>
<tr>
<td>( X_3 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
<td>0</td>
<td>( \sqrt{3} )</td>
</tr>
</tbody>
</table>

Note that this implies that many of the steady-state moments appearing in Tables 3–6 will be null because they involve odd integers for \( k \). Recall also that the highest-order moment that is controlled by DQMOM is \( k = 2n - 1 \), where \( n \) is the number of abscissas in one dimension. Thus, with \( n = 2 \), all moments up to \( m_0(3) \) will be reproduced, whereas with \( n = 3 \), all moments up to \( m_0(5) \) will be reproduced. Finally, it is important to recall that the joint Gaussian moments (eq 19) are invariant under rotations, but only the moments of order \( 2n - 1 \) and smaller that are determined from DQMOM are rotationally invariant. This implies that the steady-state weights and abscissas will be dependent on the choice of moments of order higher than \( 2n - 1 \). In other words, they will not be unique but will be dependent on the choice of \( L \).

The steady-state weights and optimal abscissas found using DQMOM with \( L = I \) are symmetric, with respect to the \( d \)-coordinate directions. Thus, it suffices to list only those in the positive quadrant. We should stress that the steady-state solutions are not dependent on the matrix \( A \) (assuming that it is full rank). Similarly, the weights and optimal abscissas for \( d = 2 \) can be found by “integrating out” the third direction for \( d = 3 \). In Table 7, the steady-state weights corresponding to the optimal abscissas for \( d = 3 \) and \( N = 8 \) are listed. Note that, for this case, the weights are equal and the optimal abscissas correspond to the corners of the unit cube. The steady-state weights and non-negative optimal abscissas for \( d = 3 \) and \( N = 27 \) are listed in Table 8. For this case, the weights are unequal but symmetric, with respect to the origin. Note that the steady-state weights and optimal abscissas can be used to estimate the steady-state moments from eq 8. Because the moment source terms are closed, all moments in the optimal moment set will be exactly predicted by eq 8 when \( L = I \), whereas moments that are not in the optimal set are not guaranteed to agree with eq 20.

The steady-state abscissas found with \( L \) defined by eq 16 will correspond to a simple rotation of the optimal abscissas. Note that all DQMOM moments of order \( 2n - 1 \) and lower will not be dependent on the choice of \( L \) and will be exactly the same as the Gaussian values (eq 20). However, the DQMOM moments of order higher than \( 2n - 1 \) will not necessarily correspond to the Gaussian values. In fact, because the optimal abscissas are symmetric with respect to the coordinate axes, the DQMOM moments found with the optimal abscissas will be closest to the Gaussian values. Although this might suggest that the optimal abscissas are the “preferred” steady-state solution, there are several reasons to reject this conclusion. First, we have shown that the optimal abscissas cannot be attained from initial conditions that are too far removed from the optimal values (see Figure 1.) Second, the FP equation is invariant under rotations, so we should not favor a set of abscissas that is dependent on an arbitrary definition of the axes. Third, for a fixed value of \( n \), we are able to exactly reproduce the moments up to order \( 2n - 1 \), which is consistent with the situation for \( d = 1 \). Thus, to control higher-order moments precisely, we should increase \( n \) rather than try to choose \( L \) in a manner that does not ensure that \( A \) is full rank for all choices of initial conditions.

**Time-Dependent Solutions with \( L = I \)**. The FP moment equations form a linear system with eigenvalues for each moment equal to \( \lambda_k = -(k_1 + k_2 + k_3) \). Thus, the moments will always relax monotonously to their steady-state values. In contrast, the DQMOM system in eq 9 is highly nonlinear in \( X \), because of the matrix \( A \). For this reason, the weights and abscissas evolve along complex trajectories that are dependent on the initial conditions \( w(0) \) and \( X(0) \), and on the definition of \( L \). Generally, our experience with solving eq 9 with \( L = I \), using a standard ordinary differential equation (ODE) solver,\(^{59}\) can be summarized as follows:

- If the initial abscissas are near the optimal abscissas in Tables 7 and 8, then eq 9 leads to a smooth relaxation to the steady-state solution. This observation is consistent with Figure 1, where it can be seen that \( A \) is nonsingular in a fairly large region around the optimal abscissas.
- Strong perturbations in the weights are easily handled by the ODE solver. This is most likely due to the fact that eq 9 for the FP equation is linear in the weights.
- If the initial abscissas are strongly perturbed from the optimal abscissas,\(^{60}\) then the relaxation to the steady-state values is not usually observed when \( L = I \). This is not surprising when one considers that even a simple rotation away from the optimal abscissas can lead to a singularity in \( A \) (see Figure 1).

In summary, we can conclude that, without the linear transformation, the DQMOM system with the optimal moment sets is not a viable method for approximating the time evolution of the (closed) moments of the FP equation. However, because the singularities are located on \((d-1)\)-dimensional subspaces (see Figure 1), this difficulty is not intrinsic to quadrature methods per se. (In other words, given the values of the optimal moments, eq 8 can almost always be inverted to determine the weights and abscissas.) Rather, it is specifically a problem with DQMOM, because eq 9 will not be well-defined when the abscissas cross a singular surface.

**Time-Dependent Solutions with the Linear-Transformation Matrix**. When the linear-transformation matrix is used with DQMOM, it is necessary to generalize the definition of the DQMOM system to include all linear combinations of the moments (see the Appendix):

\[
A \frac{\partial}{\partial t} \begin{bmatrix} w \\ Y \end{bmatrix} = M^* S^* \tag{21}
\]

where \( A \) and \( M^* \) are dependent on \( L \). In the limit where \( L = I \), eq 21 reduces to eq 9. Note that, although \( M^* \) is very sparse (see Figure 2), \( A \) is not. In this section, we will define the linear-transformation matrix using eq 16. Generally, we can note that the steady-state solution to eq 21 will correspond to the optimal abscissas when the initial abscissas are chosen such that \( L = I \).\(^{61}\) In other words, the steady-state abscissas will be different for almost every set of initial conditions. This observation should not be surprising, because we have already noted that the FP moments are rotationally invariant. Thus, each steady-state solution will correspond to a simple rotation of the optimal abscissas.
Examples of the time evolution of a set of weights and abscissas for $N = 8$ are shown in Figures 3 and 4, respectively. For clarity, the weights are initially all set to different values. The initial values of the abscissas are found by randomly rotating the optimal abscissas and then perturbing them randomly (e.g., $\pm 50\%$). The weights and abscissas can be used to compute the moments. As expected (because the moment equations are closed), the moments up to order three are reproduced exactly by DQMOM with $N = 8$. Moreover, because the stationary solution is symmetric with respect to the origin, all odd-order moments approach zero, even though they are not forced to do so explicitly by DQMOM. On the other hand, the fourth-order cross moments (such as $m(2, 1, 1)$ and $m(2, 2, 0)$) approach values that are dependent on the angle of rotation of the steady-state abscissas, with respect to the optimal abscissas. Note that this behavior is exactly as expected, because the steady-state value of $\mathbf{L}$ has no reason to approach $\mathbf{I}$, because the Gaussian moments are rotationally invariant. The results for $N = 27$ (see Figure 5) follow the same trends as those for $N = 8$; however, the computational load increases substantially, because the number of ODEs increases from 32 to 108. Finally, the evolution of the abscissas for $N = 8$ starting from values far from the optimal abscissas is shown in Figure 6. Note that the trajectories can be highly nonlinear, but eventually the abscissas end up back at the corners of the unit cube.
We have solved eq 21 successfully with many different choices for the initial conditions. Based on these simulations, we can make the following observations:

(1) The simulations are very well-behaved under simple rotations and/or with strong perturbations in the weights. In fact, the condition number for A in these cases is the same as that for the optimal abscissas.

(2) Even with large perturbations away from the optimal abscissas, we have not seen A become singular (or even very poorly conditioned).

(3) The system of ODEs in eq 21 can be very stiff when initialized with large perturbations of the abscissas. This is observed, for example, when the initial conditions place two abscissas very close to each other. The system responds by rapidly changing the weights and abscissas to reduce the stiffness.

Note that, in practice, large perturbations on the abscissas result in the moments taking on “random” initial values that normally would not be seen in most applications. Thus, the fact that eq 21 is well-behaved for reasonably large perturbations from the joint Gaussian moments is reassuring, especially when one considers that the same system with \( \mathbf{L} = \mathbf{I} \) fails under simple rotations. Whether DQMOM with the optimal moment sets and \( \mathbf{L} \) defined by eq 16 will work satisfactorily for other systems (i.e., highly non-Gaussian distributions) is an open question that deserves further investigation.

Conclusions

The success of quadrature-based moment methods for solving multivariate PBEs is dependent on our ability to identify moment sets that can be inverted to find the weights and abscissas. For any nondegenerate univariate NDF, the weights and abscissas corresponding to the integer moments are unique and can be computed with the PD algorithm. In contrast, for a multivariate NDF, there is no guarantee that a particular set of integer moments will be invertible, and even if it is, the weights can be negative and/or the abscissas may be unrealizable. In essence, multivariate problems have too many choices of moments for a given number \( N \) of quadrature nodes, and many of these lead to technical difficulties that make determination of the weights and abscissas unreliable. Thus, for quadrature methods to become a viable alternative for approximating multivariate NDFs, it critical to know how to choose robust moment sets (if they exist) for a given value of \( N \).

To overcome this difficulty, we have introduced the concept of optimal moment sets and outlined a methodology for finding such sets based on optimal abscissas. The latter correspond to the abscissas that would be used to best describe an independent joint Gaussian distribution function. Using the optimal abscissas, it is remarkable that the optimal moment set is unique for the cases examined \( (d = 1 − 3 \text{ and } n = 1 − 3) \) and, as might be expected, these sets are invariant under permutations of the indices. The connection between the optimal moments sets (valid for a particular distribution) and other multivariate NDFs is achieved through the introduction of a linear-transformation matrix. As a result of this transformation, the moments of the general NDF are mapped onto the optimal moment set, resulting in a well-defined DQMOM coefficient matrix for all possible distinct, nondegenerate abscissas. The performance of the proposed methodology was tested by applying it to a multivariate Fokker–Planck equation.

The overall conclusion from this study is that the DQMOM system defined with the optimal moment set, combined with the linear-transformation matrix, exhibits none of the singularities observed when using “non-optimal” moment sets. However, it is important to recall that optimal moment sets (as defined in this work) require \( N = n^d \) quadrature nodes, where \( n \) is the number of nodes used in one dimension and \( d \) is the number of dimensions. Mathematically this is simply a consequence of treating all \( d \) directions equally. Naturally it also should be possible to treat each direction differently \( (N = m_1 n_2 \ldots n_d) \), and we leave, as an open problem, the procedure for finding optimal moment sets for such cases. However, we can note that such cases are likely to be of great practical significance when, for example, the variance in one (or more) direction(s) is/are significantly larger than in the other directions. Furthermore, such a generalization may be useful when developing a general formulation that can handle degenerate NDFs, which were specifically excluded from consideration in this work.

Acknowledgment

We gratefully acknowledge support from U.S. National Science Foundation (CTS-0403864) and the U.S. Department of Energy.

Appendix: Linear Transformations, Moment Sets, and DQMOM

Consider a nonsingular linear transformation \( \mathbf{L} \):

\[
\mathbf{X}^* = \mathbf{LX} \leftrightarrow \begin{bmatrix} X_1' \\ X_2' \\ X_3' \end{bmatrix} = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \tag{22}
\]

Let \( m^*(\mathbf{k}) \) denote the moments of \( \mathbf{X}^* \) and \( m(\mathbf{k}) \) denote the moments of \( \mathbf{X} \) for a particular set of exponents \( \mathbf{k} = (k_1, k_2, k_3) \). Using multinomial expansions, it can be easily shown that \( m^* \) is related to \( m \) by

\[
m^*(k_1^*, k_2^*, k_3^*) = \sum_{j_1=0}^{k_1} \sum_{j_2=0}^{k_2} \sum_{j_3=0}^{k_3} \left( \begin{array}{c} k_1 \\ j_1 \\ j_2 \\ j_3 \end{array} \right) \left( \begin{array}{c} k_2 \\ j_1 \\ j_2 \\ j_3 \end{array} \right) \left( \begin{array}{c} k_3 \\ j_1 \\ j_2 \\ j_3 \end{array} \right) \times \\
\delta_{k_1,j_1+2j_2+2j_3} \delta_{k_2,j_1+2j_2+2j_3} \delta_{k_3,j_1+2j_2+2j_3} m(k_1,j_1,j_2,j_3) \tag{23}
\]

where \( \delta_{L,J} \) is the Kronecker delta. Letting \( m^* \) and \( m \) denote column vectors that contain the distinct moments in a given moment set:

\[
\begin{bmatrix} m^*(0,0,0) \\ m^*(1,0,0) \\ m^*(0,1,0) \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} m(0,0,0) \\ m(1,0,0) \\ m(0,1,0) \\ \vdots \end{bmatrix}
\]

we can observe that eq 23 defines a square transformation matrix \( (m^* = \mathbf{Mm}) \) with the following properties:

(1) \( \mathbf{M} \) is full rank.

(2) \( \mathbf{M} = \text{diag}(\mathbf{M}_0, \mathbf{M}_1, \ldots) \) is a block diagonal, where the size of the square block \( \mathbf{M}_i \) equals the number of moments of order \( \gamma \).

(3) \( \mathbf{M}_i \) will be diagonal if and only if \( \mathbf{L} \) is diagonal.

Letting \( \mathbf{m}^*_\gamma \) (\( \mathbf{m}_\gamma \)) denote the components of \( \mathbf{m}^* \) (\( \mathbf{m} \)) corresponding to moments of order \( \gamma \), it then follows that \( \mathbf{m}^*_\gamma = \mathbf{M}_\gamma \mathbf{m}_\gamma \). In other words, the moments of \( \mathbf{X}^* \) of order \( \gamma \) are a linear combination of the moments of \( \mathbf{X} \) of order \( \gamma \). Generally, unless \( \mathbf{L} \) is diagonal, a particular moment of \( \mathbf{X}^* \) of order \( \gamma \) will be a linear combination of all moments of \( \mathbf{X} \) of order \( \gamma \).
In DQ MOM, we will use the optimal moment set, which is a subset of $\mathbf{m}^i$. The corresponding moment transformation matrix $\mathbf{M}^*$ will contain a subset of the rows of $\mathbf{M}$ (i.e., one row for each moment in the optimal moment set). For example, for $d = 3$ and $N = 8$, $\mathbf{M}^*$ will have 32 rows and 56 columns, corresponding to the optimal moments up to order five, whereas for $N = 27$, it will have 108 rows and 220 columns, corresponding to the optimal moments up to order nine. Note that $\mathbf{M}^*$ will be a block diagonal and, hence, very sparse (see Figure 2). DQ MOM solves for the weights and abscissas, using

$$\mathbf{A} \frac{\partial}{\partial t} [\mathbf{w}] = \mathbf{S}$$  \hspace{1cm} (25)

where $\mathbf{A}$ and $\mathbf{S}$ are defined in terms of the moments of $\mathbf{X}$. After the linear transformation, the DQ MOM system becomes

$$\mathbf{M}^* \mathbf{A} \frac{\partial}{\partial t} [\mathbf{w}] = \mathbf{M}^* \mathbf{S}^*$$  \hspace{1cm} (26)

where $\mathbf{A}^*$ and $\mathbf{S}^*$ are defined in terms of moments of $\mathbf{X}$ up to a given order (i.e., the maximum order used to define $\mathbf{M}^*$). The new coefficient matrix $\mathbf{A} = \mathbf{M}^* \mathbf{A}^*$ is square and full rank. Moreover, $\mathbf{A}$ is dependent on the linear transformation matrix $\mathbf{L}$ through $\mathbf{M}^*$, which, in turn, will be dependent on the weights and abscissas.

**Literature Cited**


respectively, then it will be degenerate for \( n_{\text{max}} > 3 \) or \( N > 2 \) and the solution to eq 6 will not be unique. Although we will not do so here, degenerate NDFs can be identified using the canonical moments. Generally, if any of the canonical moments are equal to their maximum or minimum values, then the NDF is degenerate. Although it is not difficult to treat degenerate NDF in the context of quadrature methods, for clarity, hereinafter, we will assume that the NDF has at least a partially continuous \( d \)-dimensional support, and, thus, is nondegenerate.

(46) Certain choices of moments will minimize the condition number of \( A \), but as long as the moments are independent and the abscissas distinct, \( A \) will never be singular for \( d = 1 \).

(47) In this work, “singular region” is interpreted as distinct, nondegenerate abscissas positioned such that \( A \) is singular. It is also possible for the dynamics to lead to nondistinct abscissas (i.e., phase-space trajectory crossing) in certain cases; however, we will not consider such cases here.

(48) Although we do not need to do so here, the scaling factor can be defined component-wise: \( X_s \). As shown elsewhere, choosing \( X_s \) to be the magnitude of the largest abscissa is a good choice. Note that degenerate NDF cases would then correspond to \( X_s \to 0 \) for some \( \beta \).

(49) We shall see that certain sets of nondegenerate abscissas, corresponding to curves on the unit sphere for \( d = 3 \) and points on the unit circle for \( d = 2 \), yield a rank-deficient \( A \). Because these sets have zero measure, they will be excluded from the sets of abscissas used to define an optimal moment set.

(50) In practice, this implies that, if \( n \) is the number of nodes in one dimension, then \( N = n^d \) nodes will be needed in \( d \) dimensions. Nevertheless, in some cases, it may be useful to use different numbers of nodes for each direction: \( N = n_1 n_2 \ldots n_d \). For example, for \( d = 2 \), we could use \( n_1 = N \) and \( n_2 = 1 \), and then choose \( 2N-1 \) moments in \( X_1 \). This is essentially what was done in previous work. Similarly, with \( n_1 = 2 \) and \( n_2 = 3 \), it is possible to define an optimal moment set using the 18 moments of order five or smaller in \( X_1 \) and order three or smaller in \( X_2 \). This moment set is remarkable, because it is one of the rare examples with \( n_\alpha > 1 \) for all \( \alpha \in 1, \ldots, d \), where the number of moments is equal to the number of degrees of freedom: \(( 1 + d ) N \).

(51) It is not necessary to go above \( 2N \), because that is more than the maximum number of independent moments in any one direction of phase space.

(52) The conjectures given are based on generating hundreds of thousands of random sets for which the condition number was found to never be larger than \( 10^3 \).

(53) For \( N = 27 \), we have not observed rank deficiency under simple rotation. However, we have seen that the condition number of \( A \) can become very large, relative to its value at the optimal abscissas.

(54) Care must be taken to ensure that the negative weights are not due to numerical errors. For \( N = n^d \), we have never observed negative weights if the numerical errors due to stiffness are adequately controlled.

(55) The optimal abscissas correspond to the tensor product in \( d \) dimensions of the scaled abscissas in one dimension found for a univariate Gaussian PDF with zero mean. The latter correspond to the zeroes of the \( n \)th-order Hermite polynomial, where \( n \) is the number of abscissas.

(56) Because of the scaling properties of \( A \), the singular curves extend off the surface of the sphere. Thus, they are singular surfaces with dimension \( d-1 \).

(57) If the abscissa are nondegenerate, then \( BB^T \) should be full rank (i.e., the abscissas span the \( d \)-dimensional space.) However, to handle cases where the abscissas span a lower-dimensional space, it will be necessary to define a transformation matrix that also works in degenerate cases.

(58) The reader can easily confirm that this is the case by examining the moments in Table 6. For example, \( m(5, 2, 2) \) requires \( m(3, 2, 2) \), \( m(5, 0, 2) \), and \( m(5, 2, 0) \), which are included in the optimal set.

(59) We have used the ODE solvers ode45 and ode15s in MATLAB. Generally, the stiff solver does not improve the performance when the abscissas are strongly perturbed with \( L = I \).

(60) In this context, “strongly perturbed” means adding random normal fluctuations with zero mean and standard deviations of 50% or larger to each component of the abscissas.

(61) The steady-state solution is determined from the algebraic equation \( M^{*} S^{*} = 0 \), which is not the same as that for eq 9, because, here, \( S^{*} = 0 \) has more equations than unknowns. See the Appendix for details.