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Efficient Bandwidth Estimation in Two-dimensional Filtered Backprojection Reconstruction

Ranjan Maitra

Iowa State University, maitra@iastate.edu

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Backprojected filtering, circulant matrix, FORE, generalized cross-validation, Radon transform, risk-unbiased estimation, singular value decomposition, split violinplot

Disciplines
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Index Terms

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I. INTRODUCTION

FILTERED Backprojection (FBP) [1]–[3] is commonly used in tomographic reconstruction where the goal is to estimate an object or emitting source distribution from its degraded linear projections that have been recorded by an appropriately designed set of detectors [4]–[6]. Such scenarios arise in areas such as astronomy [7]–[9], materials science and non-destructive evaluation [10]–[14], electron microscopy [15] and tomosynthesis [16] or in object detection with security scanners [17]. A popular application is in emission tomography imaging such as Single Photon Emission Computed Tomography (SPECT) or Positron Emission Tomography (PET) [18]–[21] that forms the primary setting for this article. The challenges in emission tomography inherent in the dosimetry constraints and the Poisson distribution of the sinogram emissions have meant the development of sophisticated statistical methods [22]–[27]. Nevertheless, the computationally fast FBP is still very commonly used. Further, many of the gains associated with some of the sophisticated methods are typically in background regions and easily recovered by a quick postprocessing of the reconstructions [28], [29]. Also, three-dimensional (3D) PET reconstructions are often obtained from 2D sinograms acquired with septa in place or with Fourier Rebinning (FORE) [30]–[32]. However, FBP reconstruction is generally accompanied by smoothing that involves a bandwidth or resolution size parameter, often specified in terms of its full-width-at-half-maximum (FWHM), that must ideally be optimally set to get spatially consistent reconstructions. Similar to nonparametric function estimation in statistics, the quality of reconstruction is evaluated by, for instance, the squared error loss function [33]–[37].

Data-dependent unbiased risk estimation techniques [38], [39] – with practical modifications [40] to adjust for the extra-Poisson variation in corrected PET data – have been developed. The methodology is interpretable as a form of cross-validation (CV). Many practitioners however forego bandwidth selection schemes that involve additional steps beyond reconstruction, and instead either use a value that is fixed or visually chosen and typically undersmooths reconstructions.

The use of CV [41], [42] and the rotationally invariant Generalized CV (GCV) [43] is quite prevalent for bandwidth selection in nonparametric function estimation [44] and image restoration [45]–[47]. For moderate sample sizes, CV-obtained bandwidth parameters yield the best smoothed linear ridge and nonparametric regression estimators [48]. In image deblurring where a degraded version of the true image after convolving via a point-spread function is observed, [49] and [50] provide optimal GCV bandwidths that usually perform well [49] – howbeit see [50] for examples of undersmoothing – but are impractical to obtain in tomographic applications because they require indirect function estimation (see Section 4.1 of [49]). Consequently, Section II of this article shows that the singular value decomposition (SVD) of the reconstruction (in matrix notation) can be readily obtained from results on symmetric one-dimensional (1D) and 2D circulant matrices, which are also derived here. The Predicted Residual Sums of Squares (PRESS) are then very easily obtained in a similar spirit to [43] and practically minimized en route to FBP reconstruction to obtain the GCV-estimated bandwidth. The methodology is evaluated on simulated 2D phantom data in Section III. Our implementation and results show that GCV selection and PET reconstruction can be carried out in less than a second, achieving an integrated squared error that is very close to the ideal. Moreover, our optimal reconstructions have the maximum relative benefits at lower rates of emissions. Further, the methodology can be used to optimally select parameters in the wider class of elliptically symmetric 2D kernel smoothers. Postprocessing proposed in [28]

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further improves reconstruction quality by removing negative artifacts. Our article concludes with some discussion including areas that could benefit from further extensions of our development. This paper also has a supplement.

II. THEORY AND METHODS

A. Background and Preliminaries

Let \( y_{r\theta} \) be the attenuation-, scatter- and randoms-corrected sinogram measurement along the line of response (LOR) indexed by \((r, \theta), \ r = 1, 2, \ldots, R; \ \theta = 1, 2, \ldots, \Theta.\) Assume that the sinogram has \( n = R\Theta(> p) \) LORs. Suppose that we use FBP to reconstruct the underlying source distribution in an imaging grid of \( p \) pixels. In convolution form, the \( i \)th FBP-reconstructed pixel value, for \( i = 1, 2, \ldots, p, \) is

\[
\hat{\lambda}^h_i = \sum_{\theta=1}^\Theta \sum_{r=1}^R e_h(x_i \cos \theta + y_i \sin \theta - r)y_{r\theta}.
\]

Here, \( e_h(\cdot) \) is the convolution filter with FWHM \( h. \) The summation over \( r \) is a convolution and efficiently achieved though a series of 1D discrete Fast Fourier Transforms (FFT) and linear interpolation while the summation over \( \theta \) is the slower backprojection step. The Projection Slice Theorem and properties of the Radon transform show that there is an equivalent form of FBP called Backprojected Filtering (BPF) where the backprojection step is applied first and is followed by 2D convolution in the imaging domain [51]–[53]. BPF reconstructions have an equivalent characterization [28] as a smoothed least-squares (LS) solution in matrix form as

\[
\hat{\lambda} = S_h(K'K)^{-1}K'y,
\]

where \( y \) is the \( n \)-dimensional vector of corrected Poisson data in the sinogram domain, \( K \) is a discretized version of the Radon transform and \( S_h \) is a smoothing matrix with FWHM \( h. \) The application of \( K' \) to \( y \) is backprojection and the multiplication by \((K'K)^{-1}\) is filtering and can be done using FFTs because the matrix \((K'K)^{-1}\) is approximately 2D circulant. Moreover, if \( S_h \) is also 2D circulant, the operation \( S_h(K'K)^{-1} \) can be done in one convolution step.

Comments: We make a few remarks on our setup:

a) Smoothed FBP: A reviewer has pointed out that original FBP does not incorporate any smoothing and that our article concludes with some discussion including areas that could benefit from further extensions of our development. This paper also has a supplement.

b) Choice of \( S_h \): Another reviewer has asked about the assumption of \( S_h \) being a circulant matrix. FBP/BPF mostly use radially symmetric smoothing filters that are 2D circulant, so we do not consider this restriction to be a major limitation. At this point, we consider \( S_h \) that arises from a radially symmetric Gaussian kernel, with \((k,j)\)th element \( S_h(k,j) \propto \exp(-(k^2+j^2)/2h^2). \) (Section II-C further widens our class of reconstruction filters to include elliptically symmetric kernels.)

This paper develops an optimal method to estimate \( h \) in the setup of [1]. Leave-one-out CV (LOOCV) is often used to choose the optimal \( h \) in density estimation [35], [54]. For FBP, a LOOCV strategy would remove \( y_j \equiv y_{r\theta} \) for the \( j \)th LOR \((r, \theta), \) obtain an estimate of \( \hat{\lambda}^h \equiv \hat{\lambda}^h_{(r,\theta)} \) from the remaining LOR data \((y_{-j}), \) project it along the LOR and compare the projected (predicted) value with the observed \( y_j \) in terms of its squared error. LOOCV leads to the PRESS statistic

\[
P(h; y) = \sum_{j=1}^n [(K\hat{\lambda}^h_{-j})_j - y_j]^2,
\]

where \((K\hat{\lambda}^h_{-j})_j \) is the \( j \)th coordinate of the expected emissions predicted from the leave-\( j \)-LOR-out reconstruction \( \hat{\lambda}^h_{-j} \) (obtained from \( y_{-j} \)) and \( k'_j \hat{\lambda}^h_{-j} \) with \( k'_j \) denoting the \( j \)th row of \( K. \) Minimizing \((3) \) over \( h, \) that is, finding \( \text{arg min}_h P(h; y) \) involves multiple evaluations, for each \( h, \) of \((3), \) with each calculation requiring \( n \) reconstructions and projections (one for each left-out LOR) without the benefit of the FFT because removing a LOR damages the circulant structure of \( K'K, \) and choosing the \( h \) minimizing \((3). \) Such an approach, with time-consuming calculations for each \( h, \) is computationally impractical, so we derive an invariant version of \((3) \) that reduces to an easily computed function of \( h. \)

B. An Invariant PRESS Statistic and GCV Estimation of \( h \)

To obtain a GCV estimate of \( h, \) we first state and prove our

**Theorem 1.** Let \( U = [U_1; U_2] \) be the \( n \times n \) orthogonal matrix of the left singular vectors of \( K, \) with \( U \) partitioned into matrices \( U_1 \) and \( U_2 \) with \( p \) and \( n - p \) columns, respectively. Also, let \( \Omega_h \) be the diagonal matrix of the \( p \) eigenvalues of the circulant matrix \( S_h \) and \( c(h) = \text{trace}(\Omega_h)/(n-p). \) The GCV estimate of \( h \) for estimators of the form \((2) \) minimizes

\[
\zeta(h) = \{z_1'(I_p - \Omega_h)^2z_1 + [1 + c(h)]^2z'_2z_2\},
\]

where \( z_1 = U_1\hat{\lambda}, \) \( z_2 = U_2\hat{\lambda}, \) and \( c(h) = \text{trace}(\Omega_h)/(n-p). \)
where \( z = U' y \), \( z_1 = U'_1 y \), \( z_2 = U'_2 y \).

\[ z = U' y, \quad z_1 = U'_1 y, \quad z_2 = U'_2 y. \]

**Proof:** See Appendix A

The SVD of any \( n \times p \) (\( n > p \)) matrix is generally expensive, requiring computations on the order of at least \( 20p^3/3 \) [55]. However, the complete SVD is unnecessary to calculate (4) and obtaining \( U'_1 y \) with \( U_1 \) as in Theorem 1 is enough because \( z'_1 z_2 \) can be computed from the identity \( y' U = y' U_1 U'_1 y + y' U_2 U'_2 y = z'_1 z_1 + z'_2 z_2 \). So we devise a practical way to obtain \( U'_1 y \). Note that \( U'_1 y = D_\star^{-1} V' K' y \) where \( D_\star \) is the diagonal matrix of the \( p \) singular values of \( K \) with \( V \) being the matrix of its right singular vectors. Also, backprojection \( K' y \) is a necessary step in BPF. Our objective now is to efficiently compute \( D_\star \) and \( V' x \) for any vector \( x \). We next derive some results on the eigendecomposition of real symmetric circulant matrices.

1) **Spectral decomposition of circulant matrices:** Let \( C = \text{circ}(c_0, c_1, \ldots, c_{p-1}) \) be a circulant matrix with first row \( c = (c_0, c_1, \ldots, c_{p-1})' \) and \( \gamma_{j,p} = (1, \omega_j, \ldots, \omega_j^{p-1})' \) where \( \omega_j \) is the \( j \)th root of unity. Then [56] shows that \( d_j = c' \gamma_{j,p} \) is the \( j \)th eigenvalue of \( C \), with corresponding eigenvector \( \gamma_{j,p} \). Thus the eigenvalues of any circulant matrix can be speedily computed by using FFTs and scaling to equate the mean to \( 1 \). We next derive some results on the eigendecomposition of real symmetric circulant matrices.

**Theorem 2.** Let \( C \) be a \( p \times p \) symmetric circulant matrix. Then the eigenvalues of \( C \) are all real and the spectral decomposition of \( C = VDV' \) where, for even \( p \), \( V = [1/\sqrt{p}, M_1, \pm 1/\sqrt{p}, M_s] \) with \( M_1 = (1, 1, \ldots, 1)' \), \pm 1 = \( (1, -1, 1, -1, \ldots, 1, -1)' \), and \( M_1 \) and \( M_s \) are \( p \times p/2 \)-matrices with \( (j,k) \)th element given by \( \sqrt{2/p} \cos(2\pi k(j-1)/p) \) and \( \sqrt{2/p} \sin(2\pi (p-k)(j-1)/p) \), respectively. Further, \( D \) is the diagonal matrix of eigenvalues with \( k \)th entry

\[
d_k = c_0 + \sum_{j=1}^{p/2-1} c_j \cos \left( \frac{2\pi kj}{p} \right) + c_{p/2}(-1)^k; \quad 0 \leq k \leq p-1. \tag{5}
\]

For odd \( p \), the expression for the eigenvalues does not contain the last term. Also then, \( V \) does not contain the column vector \( \pm 1/\sqrt{p} \) and \( M_s \), \( M_s \) are \( p \times (p-1)/2 \)-matrices.

**Proof:** See Appendix B

**Corollary 3.** For a real vector \( x = (x_1, x_2, \ldots, x_p)' \), we have

1) \( \alpha = V' x \) can be computed directly from \( \beta = \Gamma' x \) because the first and \( (p/2) \)th (for \( p \) even) elements of \( \alpha \) are the real parts of the corresponding elements of \( \beta \). For \( k = 2, 3, \ldots, (p-1)/2 \), the \( k \)th element of \( \alpha \) is the real part of the scaled sum of the \( k \)th and the \( (p-k+2) \)th elements of \( \beta \) while the \( (p-k+2) \)th element of \( \alpha \) is the imaginary part of the scaled difference of the \( k \)th and the \( (p-k+2) \)th elements of \( \beta \). In both cases, the scaling factor is \( \sqrt{2} \). Also, here \( \lfloor \xi \rfloor \) is the smallest integer that is no more than \( \xi \).

2) Let \( \psi_1 = (\sqrt{2}x_1, \sqrt{2}x_2, \ldots, \sqrt{2}x_{p/2+1}, 0') \), where \( 0 \) is a vector of 0’s and \( \mathbb{I}[\cdot] \) is the indicator function. Also, let \( \psi_2 = (0, x_{p/2+2}, x_{p/2+3}, \ldots, x_p)' \). Then each element of \( V' x \) is the sum of the real and imaginary parts of the corresponding elements of \( \Gamma_1' \psi_1 / \sqrt{2} \) and \( \Gamma_2' \psi_2 / \sqrt{2} \), respectively.

**Proof:** Part 1 follows from the proof of Theorem 2 while part 2 follows by direct substitution.

Corollary 3 means that both \( V' x \) and \( V x \) can be efficiently computed using FFTs. We now provide additional reductions on 2D circulant matrices needed to calculate (4) for BPF.

2) **Spectral Decomposition of 2D Circulant Matrices:**

**Definition 4.** A 2D circulant matrix or, alternatively, a block-circulant-circulant-block (BCCB) matrix is a \( pq \times pq \)-dimensional matrix \( C \) with \( p \) circulant blocks of \( q \)-dimensional circulant matrices. Thus, \( C = \text{circ}(C^{(0)}, C^{(1)}, \ldots, C^{(p-1)}) \), where each \( C^{(i)} = \text{circ}(c_0^{(i)}, c_1^{(i)}, \ldots, c_{q-1}^{(i)}) \).

Note that a symmetric BCCB matrix necessarily has symmetric blocks of symmetric circulant matrices. We now state a result on the eigen-decomposition of such matrices.

**Theorem 5.** Let \( \{\gamma_{k,p}; k = 1, 2, \ldots, p\} \) and \( \{\gamma_{k,q}; k = 1, 2, \ldots, q\} \) be as in Section II-B1. The \( (k,j) \)th eigenvalue of a BCCB matrix \( C \) is \( d_{k,j} = \sum_{l=0}^{p-1} \sum_{m=0}^{q-1} c_{l,m}^{(i)} \omega_{k,p}^{m} \omega_{j,q}^{n} \) with eigenvector \( \gamma_{k,p} \otimes \gamma_{j,q} \). Then the spectral decomposition of \( C = (\Gamma_p \otimes \Gamma_q) D (\Gamma_p \otimes \Gamma_q)' \) where \( D \) is the diagonal matrix of eigenvalues \( \{d_{k,j}; j = 1, 2, \ldots, q, k = 1, 2, \ldots, p\} \).

**Proof:** The result follows by direct substitution and the fact that \( \gamma_{k,p} \) and \( \gamma_{k,q} \) are eigenvectors of \( p \times p \) and \( q \times q \) 1D circulant matrices, respectively.

Theorem 5 means that 2D FFTs can be used for eigendecomposition of a BCCB matrix \( C \). More pertinent, the eigenvalues \( d_{k,j} \) are scaled versions of the 2D FFT of \( C \), with scaling factor that equates the mean \( d_{k,j} \) to the first element of \( C \). We now derive results for symmetric BCCB matrices.
Corollary 6. Let $V_p$ and $V_q$ be as in Theorem 2. Then the spectral decomposition of a symmetric BCCB matrix $C$ is given by $C = (V_p \otimes V_q)D(V_p \otimes V_q)'$, with $D$ as in Theorem 3.

Proof: Standard results on real symmetric matrices guarantee such a real-valued spectral decomposition. Replacing $\Gamma_p$ by $V_p$ and $\Gamma_q$ by $V_q$ in Theorem 3 yields the result.

Corollary 6 means that for BCCB matrices, $V'x$ can be computed for any $x$ using forward FFTs. Hence, $U^*_Dy$ of Theorem 1 is easily calculated in a one-time calculation that can be used together with the bandwidth-dependent parts of (4) to find the minimum. These latter calculations all involve linear operations on the FFT results and can be speedily executed.

C. Extension to Elliptically Symmetric Smoothing Kernels

Most 2D FBP/BPF reconstruction filters are radially symmetric. But the wider class of elliptically symmetric kernels, such as the 2D Gaussian kernel with parameters $(h_1, h_2, \rho)$

$$S_{h_1, h_2, \rho}(k, j) \propto \exp \left\{ -\frac{1}{1-\rho^2} \left( \frac{k^2}{h_1^2} + \frac{j^2}{h_2^2} - 2\rho \frac{kj}{h_1 h_2} \right) \right\},$$

provide greater flexibility because they allow for differential smoothness along different directions and can better accommodate the natural orientation of elongated structures. However, visually selecting optimal parameters for such kernels can be taxing because of the larger set of parameters involved. Unlike FBP that uses 1D filtering, BPF uses 2D filtering and so it is easy to incorporate such kernels. Our development of Section II-B extends immediately, with $h$ in (4) replaced by $h_1, h_2, \rho$ while optimizing (4), making it possible to use elliptically symmetric smoothing kernels in BPF reconstruction.

D. Overview of the GCV Bandwidth Selector

We summarize here the steps of our method:

1. **Corrected sinogram data.** Get sinogram data $y$ after corrections for attenuation, scatter, randoms and so on.

2. **Backprojection.** Backproject $y \to \hat{\lambda} = K'\hat{y}$.

3. **Optimal bandwidth selection.** Apply the following steps:
   a) Obtain $D_k^2 = D$ and (nominally) $V = V_p \otimes V_q$ for the approximately circulant $K'K$ following Theorem 3 and Corollary 6. Use forward FFTs to calculate $V'\hat{\lambda}$ and get $z_1 = U'y = D^{-1}_r V'\hat{\lambda}$. Also, obtain $z_2^*z_2 = y'y - z_1^*z_1$.
   b) For each $h$, obtain the eigenvalues, and hence $\Omega_h$, of the circulant smoothing matrix $S_h$, using Theorem 5. Calculate $\zeta(h)$ in (4). Then $h_G = \arg\min_h \zeta(h)$ is the GCV-estimated $h$.

4. **Filtering.** The optimal GCV reconstruction is $\hat{\lambda}^{h_G} = S_{h_G}(K'K)^{-1}\hat{\lambda}$.

Our GCV selection method only needs the additional Step 3 beyond BPF reconstruction. But Step 3 is a one-time calculation, done by FFT, as also is Step 3 unless the smoothing matrix is specified in the Fourier domain, in which case $\Omega_h$ is provided. Further, our algorithm outlined above details the method for radially symmetric smoothing kernels. For elliptically-symmetric kernels as in Section II-C, the $h$ is replaced by the vector $(h_1, h_2, \rho)$ in Steps 3b and 4.

A reviewer asked about $z_1$ and $z_2$. Our development shows that $z_1$ to be a weighted version of the forward FFT of the backprojected sinogram data, with the weights given by the square root of the ramp filter. Further $z_2^*z_2$ is the residual sum of squares after removing the effect of the projection of $z_1 = U_1y$ from the corrected sinogram data $y$. Separately, as also pointed out by the reviewer, the same matrices diagonalize the circulant matrices $S_h$ and $K'K$ since their orders are the same.

III. PERFORMANCE EVALUATIONS

A. Experimental Setup

The performance of our GCV approach was explored in a series of simulated but realistic 2D PET experiments. Our setup used the specifications and the sixth slice of the digitized Hofmann [57] phantom (Figure 1a) on a discretized imaging domain having $128 \times 128$ pixels of dimension $2.1$ mm each. Our sinogram domain had $128 \times 320$ distance-angle bins (LORs) of size $2.1mm \times \pi/320$ radians. Pseudo-random Poisson realizations were simulated in the sinogram domain with mean intensity given by the corresponding discretized Radon transform of the phantom. The total expected counts $\Lambda$ varied over 9 distinct equi-spaced (on a log$_2$ scale) values between $10^5$ and $10^6$ counts. Therefore, $\Lambda$ ranged from the very low (about 0.61 counts per pixel) to the moderately high (61 counts per pixel) and matched the range of values typically seen in individual scans in dynamic 2D PET studies [53]. Our first set of evaluations used a radially symmetric Gaussian kernel $S_h$ with FWHM $h$. Subsequent evaluations used elliptically symmetric Gaussian kernels with parameters $h_1, h_2, \rho$. We use “BPFe” to denote BPF reconstructions with elliptically symmetric kernels and “GCVe” to denote GCV estimated parameters in these settings. We also evaluated performance in applying reducing negative artifacts as per [28] – we add “+” in the nomenclature to denote this additional postprocessing step. For each simulated sinogram dataset, we obtained the optimal BPF, BPFe, BPF+ and BPF+ reconstructions and the corresponding optimal bandwidths as follows: for the BPF reconstruction $\hat{\lambda}^h$ using a radially symmetric Gaussian filter with FWHM $h$, we calculated the Root Mean Squared Error (RMSE) $\hat{R}_h = \| \hat{\lambda}^h - \lambda \| / \sqrt{n}$, with $\lambda$ the true source distribution (the
Hoffman [57] phantom). The $h_O$ corresponding to the BPF reconstruction that minimizes the RMSE (i.e., the $h_O$ such that $R_{h_O} \leq R_h$ for all $h \neq h_O$) is our true optimal FWHM for the simulated sinogram dataset. Similar optimal FWHM parameters and gold standard reconstructions were obtained for BPFe, BPF+ and BPFe+ reconstructions (note that BPFe and BPFe+ have trivariate smoothing parameters.) We evaluated performance of reconstructions obtained using our GCV-estimated procedure ($h_G$) in terms of the RMSE and compared them for BPF and BPF+ reconstructions with corresponding calculations obtained using the MRUE- and MRUP-estimated [39], [40] bandwidths $h_E$ and $h_{P_E}$, respectively. We also evaluated performance of each reconstruction in terms of its RMSE efficiency relative to the gold standard reconstruction obtained using $h_O$, that is, we calculated RMSE efficiency for a BPF reconstruction with filter resolution $h$ as $R_{h}/R_{h_O}$. Corresponding evaluations were done for BPFe, BPF+ and BPFe+ reconstructions, with smoothing parameters in BPFe and BPFe+ optimized over trivariate sets. Reducing negativity artifacts does not involve choosing a $h$ beyond that chosen for BPF or BPFe; however the optimal BPF+ or BPFe+ bandwidths may be different from the optimal BPF and BPFe ones. We simulated 1000 sinogram datasets and evaluated reconstruction performance using the different methods.

**B. Results**

1) **Illustrative Examples:** We first illustrate performance on a sample simulated sinogram realization with $\Lambda = 10^5$.

   a) **BPF reconstruction:** Figure 1b provides the “gold standard” BPF/FBP reconstruction obtained using $h_O$. BPFe, BPF+ and BPFe+ reconstructions (note that BPFe and BPFe+ have trivariate smoothing parameters.) We evaluated performance of reconstructions obtained using our GCV-estimated procedure ($h_G$) in terms of the RMSE and compared them for BPF and BPF+ reconstructions with corresponding calculations obtained using the MRUE- and MRUP-estimated [39], [40] bandwidths $h_E$ and $h_{P_E}$, respectively. We also evaluated performance of each reconstruction in terms of its RMSE efficiency relative to the gold standard reconstruction obtained using $h_O$, that is, we calculated RMSE efficiency for a BPF reconstruction with filter resolution $h$ as $R_{h}/R_{h_O}$. Corresponding evaluations were done for BPFe, BPF+ and BPFe+ reconstructions, with smoothing parameters in BPFe and BPFe+ optimized over trivariate sets. Reducing negativity artifacts does not involve choosing a $h$ beyond that chosen for BPF or BPFe; however the optimal BPF+ or BPFe+ bandwidths may be different from the optimal BPF and BPFe ones. We simulated 1000 sinogram datasets and evaluated reconstruction performance using the different methods.

   b) **BPFe reconstruction:** We next illustrate GCVe’s performance in choosing optimal parameters for BPFe reconstructions. Figure 2c shows reconstructions obtained using the true optimal and the GCVe-selected parameters. The reconstruction RMSE (Figure 2c) of $8.376 \times 10^{-5}$ obtained using BPFe with GCVe even marginally outperforms BPF reconstruction using $h_O$ and compares favorably with the true optimal RMSE of $8.289 \times 10^{-5}$. The illustration shows some undersmoothing with GCVe and scope for improved parameter estimates, but the wider class of elliptically symmetric kernels throws opens the possibility for further improvements to reconstruction.

   c) **Reconstructions with reduced negative artifacts:** We also explored performance in BPF+ and BPFe+ reconstructions, having gold standards as per Figure 3d ($h_{O+} = 2.766$; RMSE $= 7.873 \times 10^{-5}$) and Figure 3d ($h_1 = 3.818, h_2 = 2.216, \rho = -0.035$; RMSE $= 7.831 \times 10^{-5}$), respectively. For BPF+, the GCV-estimated bandwidth of $h = 3.279$ yields the reconstruction of Figure 3d (RMSE$ = 7.976 \times 10^{-5}$) while MRUP provides the BPF+ reconstruction of Figure 3d (RMSE$ = 1.008 \times 10^{-4}$). For brevity of display, we forego discussing BPF+ reconstructions done with MRUE-selected bandwidths, noting simply that they also improve over BPF under BPF+ (with RMSE$ = 8.646 \times 10^{-5}$ in this example) but that improvement falls far short of that obtained using GCVe. Figure 3d also shows improvement of BPFe+ over BPFe (RMSE $= 7.968 \times 10^{-5}$) when negative
(a) BPF+ Gold standard  (b) GCV+  (c) MRUP+  (d) BPFe+ Gold standard  (e) GCVe+

Fig. 3: (a-c) BPF+ reconstructions using the (a) optimal, (b) GCV- and (c) MRUP-estimated bandwidths. (d, e) BPFe+ reconstructions using the (d) optimal and (e) GCVe-estimated parameters.

artifacts are eliminated using [28], but the improvement is very marginal. Note that [28] reduces negative artifacts using a radially symmetric filter – an alternative approach that allows for greater flexibility in smoothing out negative values may be more appropriate.

2) Large-scale Simulation Study: We report results of our large-scale simulation study on the performance (in terms of RMSE) of the different bandwidth selection and reconstruction methods and their distribution for different values of $\Lambda$. Reconstructions using MRU bandwidths have RMSEs substantially higher than those using the optimal or GCVe-estimated bandwidths (Figure 4a) and certainly for lower values of $\Lambda$, so we display performance of these estimators separately in Figure 4b in order to attain finer granularity for displays involving our methods. Figure 4a displays RMSEs of BPF, BPFe, BPF+ and BPFe+ reconstructions obtained with GCV and the corresponding true optimal bandwidth parameters. The BPFe reconstructions using the GCVe-estimated bandwidths have similar, if not lower RMSEs, to those obtained with the gold standard BPF reconstructions. Reducing negative artifacts [28] improves the quality of BPF or BPFe reconstructions that is more substantial at higher $\Lambda$-values. But the improvement with using GCVe-estimated elliptically symmetric filters over GCVe-estimated radially symmetric filters tapers off at higher total expected counts. However, the optimal BPFe estimator improves reconstruction quality in terms of having lower RMSEs over the gold standard BPF reconstructions. Thus, the performance of GCVe-estimated reconstruction relative to the gold standard BPFe is not as strong as that of the GCV-estimated reconstruction relative to the BPF gold standard. This observation is also supported by the relative RMSE efficiency displays in Figure 4c. This may be because, as per the table in Figure 2c of our illustrative example, the bandwidth parameter sets are quite different than the true optimal BPFe parameters. Nevertheless, Figure 4a shows that any of the GCV methods out-performs the MRUE methods, especially at low total expected counts, both in terms of raw RMSE (Figure 4b) and relative RMSE efficiency (Figure 4c). Indeed, the relative RMSE efficiencies are almost always above 0.95 for the GCV methods. However, the MRU reconstructions are rather poor, especially at lower values of $\Lambda$. The MRUP results reported here are a bit more pessimistic than those over limited $\Lambda$ reported in [39] and [40]. Interestingly and contrary to their results, for larger (but not smaller) values of $\Lambda$, MRUE outperforms MRUP: comparison with their computer code indicates that the optimal bandwidths are often attained outside their chosen ranges for several cases. Reducing negative artifacts as per [28] improves MRUE reconstructions slightly – we omit these RMSEs in Figures 4b and 4c for clarity of display. The methods of [28] degrades MRUE reconstructions for lower $\Lambda$-values but with increasing $\Lambda$, MRUP+ generally performs the best among all MRUE estimates. The rate of efficiency of reconstructions with increasing $\Lambda$ obtained using GCVe-selected bandwidths is lower than either MRUE or MRUP, but the implications are unclear, given its superior performance at all $\Lambda$. The results point to the ability of the GCVe-estimated bandwidths in obtaining improved reconstructions in situations with low and high expected total emissions.
Fig. 4: (a) Split violin plot distributions against total expected counts ($\Lambda$) of the 1000 RMSEs for reconstructions using GCV-estimated (left violin lobe) and the corresponding gold standard (right lobe) reconstruction. For each $\Lambda$-value, violins are in the order of BPF, BPFe, BPF+ and BPFe+ reconstructions. Bars on each split violin display the upper, median and lower quartiles of the RMSEs. (b) RMSEs of MRUE, MRUP and MRUP+ reconstructions and (c) RMSEs of all reconstructions relative to the corresponding gold standard for different total expected counts using different bandwidth selection and reconstruction methods.
C. Some Theoretical Analysis of the GCV Selector

We now discuss some theoretical properties of the reconstructions obtained using the GCV-selected bandwidth. Because our primary setting for investigating bandwidth selection in this article is PET and because of the additional complication provided by the Poisson distribution of the emissions, our investigation is in the context of an idealized emission tomography experiment. Suppose that we have \( y \) realized from an inhomogeneous Poisson Process with \( E(y) = \mu = K\lambda \) and \( \Lambda = \sum_{d,t} \mu_{d,t} \). Our interest is in estimating \( f = \lambda / \Lambda \), for which we propose the estimator \( \hat{f}^h = \lambda^h / \Lambda \). As in [40], define the loss function in the estimation and prediction domains to be \( L_e(\hat{f}^h, f) = \| \hat{f}^h - f \|^2 \) and \( L_P(\hat{\mu}^h, \mu) = \Lambda^{-2} \| \hat{\mu}^h - \mu \|^2 \), respectively, with corresponding risk functions as \( R_e(\hat{f}^h, f) \) and \( R_P(\hat{\mu}^h, \mu) \). From the SVD of \( K = U_1 D \Sigma V \) (where \( U_1, U_1 \) when \( n \geq p \)), we have \( K'K = VD_\Sigma^2V' \). Also \( S_h = V\Omega_hV' \) because it is circulant, so that \( S_h^{-1}K'K^{-1} = V\Omega_h D_\Sigma^{-1}U_1' \) and \( K\Sigma_h(K'K)^{-1}K' = U_1\Omega_h U_1' \). Then

\[
\begin{align*}
R_P(\hat{\mu}^h, \mu) &= -2E[\|KS_h(K'K)^{-1}K'y - KL\lambda\|^2] \\
&= -2E[\|U_1\Omega_h U_1'(y - \mu) + KS_h\lambda - K\lambda\|^2] \\
&= -2E[\|U_1\Omega_h U_1'(y - \mu) - U_1D\Sigma(I_p - \Omega_h)V'\lambda\|^2] \\
&= -2E[tr((y - \mu)'U_1\Omega_h U_1'(y - \mu)] \\
&= -2E[tr((y - \mu)'U_1\Omega_h U_1'\Omega_h D_\Sigma (I_p - \Omega_h)V') + \lambda - 2tr(\lambda'V(I_p - \Omega_h)D_\Sigma^2V')].
\end{align*}
\]

Interchanging the expectation and the trace operators, the second term vanishes because \( E'y = \mu \). Also using the property that the trace of the product of two conformable matrices is the trace of their product in the reverse order (as long as they are also conformable in the reverse order), the first term equals \( \lambda - 2tr(VD_\Sigma^2\Omega_h U_1'U_1\Omega_h D_\Sigma^2V'S) \) and then

\[
R_P(\hat{\mu}^h, \mu) = -2tr(U_1\Omega_h U_1'\Sigma + (\lambda'V(I_p - \Omega_h)D_\Sigma^2V')).
\]

Under the idealized conditions of this section, \( \Sigma = diag(\mu) \) is the dispersion matrix of \( y \). Now \( R_e(\hat{f}^h, f) = \Lambda^{-2}E[\hat{f}^h - f]^2 = \Lambda^{-2}E[\|V\Omega_h D_\Sigma^2U_1'y - \lambda\|^2] \) and using similar arguments as for \( R_P(\hat{\mu}^h, \mu) \) yields

\[
R_e(\hat{f}^h, f) = \Lambda^{-2}tr(U_1D_\Sigma^2U_1'\Sigma + \lambda'V(I_p - \Omega_h)D_\Sigma^2V') = \Lambda^{-2}tr(D_\Sigma^2[I_2\Sigma U_1'U_1 + D_\Sigma^2(I_p - \Omega_h)D_\Sigma^2V']).
\]

Exploiting the diagonality of \( D_\Sigma \) and the nonnegative definiteness of the matrices inside the trace operator yields that \( R_e(\hat{f}^h, f) \leq tr(D_\Sigma^2)R_P(\hat{\mu}^h, \mu) \). Using similar arguments, \( R_P(\hat{\mu}^h, \mu) \leq tr(D_\Sigma^2)R_e(\hat{f}^h, f) \) so that both risks are minimized at the same \( h \). From Theorem [1]

\[
\Lambda^{-2}E\zeta(h) = \Lambda^{-2}tr[I_2\Sigma U_1'U_1 + \lambda'V(I_p - \Omega_h)^2D_\Sigma^2V' + \lambda + (1+c(h))D_\Sigma^2V'] \\
= \Lambda^{-2}tr\{(1+c(h))^2tr\Sigma - \{2c(h) + c^2(h)trU_1'\Sigma U_1 - 2tr\Omega_h U_1'U_1\} \} \\
= \Lambda^{-2}\{\{1+c(h))^2\vartheta_n,p - \{2c(h) + c^2(h)\}tr\varphi_n,p - 2tr\Omega_h \varphi_{n,p} \},
\]

where \( \vartheta_n,p = \lambda^{-1}tr\Sigma \) and the matrix \( \varphi_{n,p} = \lambda^{-1}U_1'\Sigma U_1 \) are both free of \( \Lambda \). Thus, as \( \Lambda \to \infty \),

\[
\frac{E\zeta(h) - R_P(\hat{\mu}^h, \mu)}{R_P(\hat{\mu}^h, \mu)} \to 0.
\]

For \( n >> p \), we have \( E\zeta'(h) \approx R_P(\hat{\mu}^h, \mu) - \frac{d}{\Lambda} tr\Omega_h \varphi_{n,p} \) so that for large \( \Lambda \), the risk has an inflexion point close to the bandwidth optimizing \( E\zeta(h) \). (To see this, consider the example of using a Butterworth filter for which the \( \nu \)th diagonal element of \( \Omega_h \) is \( (1 + h \| \nu \|^{-1}) \). This discussion provides some theoretical understanding of GCV’s good performance in selecting \( h \) for all values of \( \Lambda \) when \( n >> p \) as is the case with emission tomography or in our experiments.

A reviewer wondered about performance when \( n >> p \) is not satisfied. The supplement shows results on our large-scale simulation study done for cases when \( K'K \) is nearly ill-conditioned, and also not as well-conditioned as in our experiments in Section [III-B2]. Interestingly the GCV-estimated BPF methods do not do well relative to the optimal, but the GCV-estimated BPF+ methods continue to do well. This phenomenon needs more study.

IV. Discussion

This paper developed a computationally efficient and practical approach to selecting the filter resolution size in 2D FBP reconstructions. Our approach hinges on implementing FBP through its equivalent BPF form, uses GCV and outperforms available adaptive methods in simulated PET studies, irrespective of the total expected rates of emissions. The approach also has the ability to incorporate a wider class of elliptically symmetric 2D reconstruction filters with the potential for further improving performance. In general, FBP is more commonly used than BPF, but this is perhaps because of its origins in X-ray computed tomography where reconstruction can begin along LORs for a given projection angle even while data along other
projection angles are being acquired. However, in emission tomography, the data need to be completely acquired in the given time interval before reconstruction can begin so using BPF may not be much of a slower alternative to FBP. The easy estimation of the filter resolution size and its good performance even at lower emissions rates (which translates to lower signal-to-noise ratio for other applications) potentially makes it desirable to also use BPF in applications where reconstruction in the form of the 1D filtering step can be begun synchronous with data acquisition at other projection angles also. This would hold especially if the waiting time for data acquisition at all angles is more than compensated by the increased reconstruction accuracy afforded by GCV selection of the bandwidth. Methods speeding up backprojection [59] can further reduce the cost for using BPF.

There are a number of extensions that could benefit from our development. For instance, adopting an improved windowing function for windowed FBP has been shown [60] to improve reconstruction accuracy over FBP. It would be instructive to see the performance of GCV-selected bandwidths in such scenarios. Separately, the FORE algorithms [30] recast the 3D PET reconstruction problem into several 2D reconstructions. [61] showed that FORE reconstructions using ordered subsets expectation maximization (FORE+OSEM) are out-performed by the attenuation-weighted ordered subsets expectation maximization (FORE+AWOSEM) refinement and FORE+FBP reconstructions. It would be worth investigating whether FORE+FBP reconstructions can be further improved by using BPF in place of FBP, and with optimal GCV-estimated bandwidth. It would also be worth evaluating whether BPF+reconstructions with optimal GCV-estimated bandwidths can improve estimates of kinetic model parameters in dynamic PET imaging where FBP reconstructions are the norm. There is scope for optimism here, given our method’s good performance for both lower and higher radiotracer uptake values. Nevertheless, this performance needs to be evaluated and calibrated in such contexts. Finally, another set of potential extensions could make possible the practical implementation of penalized reconstruction methods [50] in BPF or for regularizing reconstructions obtained using [22], [23], [27]. Thus, we see that while the methods developed here show promise in improving 2D FBP/BPF reconstruction by improved estimation of the filter resolution size using GCV, issues that merit further attention remain.

APPENDIX

A. Proof of Theorem 7

The development and proof of the theorem closely mirror that of estimating the ridge regression parameter in [43]. Define the $(n-1)$ x $p$ matrix $K_{-j}$ to be $K$ with the $j$th row $k_j$ removed. So, $K^\prime = (K^\prime_{-j}, k_j)$. We will use the following equalities: $K^\prime_{-j}K_{-j} = K^\prime K - k_j k_j^\prime$ and $K_{-j}y_{-j} = Ky - k_j y_j$ and $\hat{\lambda}_j^h = S_h(K^\prime_{-j}K_{-j})^{-1}K_{-j}y_{-j}$. The LOOCV mean squared error (CVMSE) is $\tau(h) = \frac{1}{n} \sum_{j=1}^{n} (k_j^\prime \hat{\lambda}_j^h - y_j)^2$. Let $\hat{\lambda} = Q_k K^\prime y$ be the (unsmoothed) LS reconstruction, with $Q_k \equiv (K^\prime K)^{-1}$ in order to compress expressions. Using the Sherman-Morrison-Woodbury theorem, it follows that

$$k_j^\prime \hat{\lambda}_{-j} - y_j = k_j^\prime S_h \left[ Q_k + \frac{Q_k k_j k_j^\prime Q_k}{1 - k_j^\prime Q_k k_j} \right] (K^\prime y - k_j y_j) - y_j$$

$$= k_j^\prime \hat{\lambda}_j + k_j^\prime S_h k_j k_j^\prime \hat{\lambda}_j - k_j^\prime S_h k_j y_j - \frac{k_j^\prime S_h k_j k_j^\prime Q_k k_j y_j}{1 - k_j^\prime Q_k k_j} - y_j$$

$$= (k_j^\prime \hat{\lambda}_j - y_j) + \frac{\Gamma_{j,h}}{1 - \Gamma_{j,j}} (k_j^\prime \hat{\lambda}_j - y_j)$$

where $\Gamma_{j,j,h} = k_j^\prime S_h Q_k k_j$ and $\Gamma_{j,j} = k_j^\prime Q_k k_j$. Let $\Delta_h$ be the diagonal matrix with $\Gamma_{j,j,h}/(1 - \Gamma_{j,j})$ as the $(j,j)$th element. Then, using the above, the CVMSE reduces to

$$\tau(h) = \frac{1}{n} \left\{ y' \left[ I_n - K S_h Q_k K^\prime \right]' \left[ I_n - K S_h Q_k K^\prime \right] \hat{\lambda} + 2 y' \left[ I_n - K S_h Q_k K^\prime \right] \Delta_h \left[ I_n - K Q_k K^\prime \right] y \right\}$$

$$+ y' \left[ I_n - K Q_k K^\prime \right]' \Delta_h^2 \left[ I_n - K Q_k K^\prime \right] y$$

(6)

Let $D_{\bullet}$ be the diagonal matrix of the square root of the non-zero eigenvalues of $K^\prime K$. Let $K = UD^V$ be the SVD of $K$ with $U$ as in the theorem statement, $D$ be $D_{\bullet}$ augmented row-wise by an $(n-p) \times p$ matrix of zeros, and $V$ have columns containing the right singular vectors of $K$. Further, let $W$ be the corresponding unitary matrix that diagonalizes any 1D (see [56]) or 2D (see Theorem 5) circulant matrix. Under the rotated generalized linear model having observations $\hat{y} = W U^\prime y$, the reconstruction problem reformulates to estimating $\lambda$ from $E(\hat{y}) = W D^2 V \lambda \equiv \hat{K} \lambda$, where $\hat{K} = WD^\prime U^\prime$. Now $K^\prime \hat{K} = V D^2 U^\prime V$ so that $\hat{K} (K^\prime \hat{K})^{-1} \hat{K}'$ and $K S_h (K^\prime \hat{K})^{-1} \hat{K}'$ are both circulant, with each having exactly positive and non-zero eigenvalues given by the diagonal elements of $I_p$ and $\Omega_h$, respectively. Consequently $(I_n - \hat{K} (K^\prime \hat{K})^{-1} \hat{K}') = WD_{(0_p, I_{n-p})} W^\ast$ and $(I_n - K S_h (K^\prime \hat{K})^{-1} \hat{K}') = WD_{(I_p - \Omega_h, I_{n-p})} W^\ast$ where $W^\ast$ is the complex conjugate transpose of $W$, $0_p$ is a $p \times p$ matrix of zeros and $D(A, B)$ denotes a block-diagonal matrix with matrices $A$ and $B$ in the diagonals. Therefore, both $K S_h (K^\prime \hat{K})^{-1} \hat{K}'$ and $(I - \hat{K} (K^\prime \hat{K})^{-1} \hat{K}')$ are circulant (the latter is also idempotent) with constant diagonals. In the rotated framework, $\Gamma_{j,j,h} = tr(\Omega_h)/n$ (note that $tr(\Omega_h)$ is $p$ times any diagonal element of $S_h$) while $1 - \Gamma_{j,j} = (n-p)/n$, and so $\Delta_h = c(h) I_n$. In the rotated framework, we consider the three terms in (6) individually. The first term reduces to

$$\hat{y}' \left[ I_n - K S_h (K^\prime \hat{K})^{-1} \hat{K}' \right]' \left[ I_n - K S_h (K^\prime \hat{K})^{-1} \hat{K}' \right] \hat{\lambda} \equiv y' UD^2_{(I_p - \Omega_h, I_{n-p})} U^\prime y = z_1' (I_p - \Omega_h)^2 z_1 + z_2' z_2$$
while the second term
\[
2\gamma' |I_n - K S_h (K' K)^{-1} K'| \Delta_h |I_n - K (K' K)^{-1} K'| y = 2c(h) y' U D (I_p - \Omega, I_n - p) D (0, p, I_n - p) U y = 2c(h) z_2^2 z_2
\]
with \(0_{r,s}\) being the \(r \times s\) matrix of zeroes. The third term
\[
\gamma' |I_n - K (K' K)^{-1} K'| \Delta_h |I_n - K (K' K)^{-1} K'| y = c^2(h) y' U D (0, p, I_n - p) U' y = c^2(h) z_2^2 z_2.
\]

Theorem 1 follows, after scaling all sides by \(n\). \(\square\)

**B. Proof of Theorem 2**

Let \(\ell\) be the integer part of \((p + 1)/2\). Let \(c = \{c_0, c_1, c_2, \ldots, c_{\ell-1}, c_{\ell}, c_{\ell+1}, \ldots, c_1\}\) be the first row of \(C\) for even \(p\); the middle term \(c_{\ell}\) is absent for odd \(p\). Writing the \(k\)th of the \(p\) complex roots of unity as \(\exp \{i 2\pi k/p\} = \cos(2\pi k/p) + i \sin(2\pi k/p)\), the \(k\)th eigenvalue of \(C\) is \(d_k = \sum_{j=0}^{p-1} c_j \omega_k^j = c_0 + \sum_{j=1}^{p/2} c_j \cos(2\pi jk/p) + c_{p/2}(-1)^k; 0 \leq k \leq p - 1\), with the last term in the summation absent for \(p\) odd. From \[\text{or directly, an eigenvector corresponding to } d_k = \gamma(\omega_k) = \{1, \omega_k, \omega_k^2, \ldots, \omega_k^{p-1}\}\). Further, \(d_k = d_{p-k}\) for \(k = 1, 2, \ldots, \ell - 1\). This means that any symmetric circulant matrix has two (only one for \(p\) odd) real eigenvalues of algebraic multiplicity one with eigenvectors given, up to constant division, by \(1 = \{1, 1, \ldots, 1\}\) and (for \(p\) even) \(+1 = \{-1, -1, 1, -1, \ldots, -1\}\). There are at most \(\ell - 1\) distinct eigenvalues of algebraic multiplicity \(2\); for \(1 \leq k \leq \ell - 1\), the eigenvectors corresponding to \(d_k = \gamma(\omega_k)\) and \(\gamma(\bar{\omega}_k)\), where \(\bar{\omega}_k\) is the complex conjugate of \(\omega_k\). Therefore, \(\gamma(\omega_k) + \gamma(\bar{\omega}_k)\) and \(i(\gamma(\omega_k) - \gamma(\bar{\omega}_k))\) are also distinct (and real) eigenvectors that correspond to \(d_k\). Theorem 2 follows. \(\square\)

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**REFERENCES**


Fig. S-1: Split violin plot distributions against total expected counts (Λ) of the 1000 RMSEs for reconstructions using GCV-estimated (left violin lobe) and the corresponding gold standard (right lobe) reconstructions for simulation experiments with (a) $128 \times 129$ and (b) $128 \times 160$ distance-angle pairs. The imaging domain had $128 \times 128$ pixels.