FAST STEERABLE PRINCIPAL COMPONENT ANALYSIS

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ABSTRACT
We introduce an algorithm that efficiently and accurately performs principal component analysis (PCA) for a large set of two-dimensional images, and, for each image, the set of its uniform rotations in the plane and its reflection. For a dataset consisting of \( n \) images of size \( L \times L \) pixels, the computational complexity of our algorithm is \( O(nL^3 + L^4) \) which is \( L \) times faster than existing algorithms. The new algorithm computes the Fourier-Bessel expansion coefficients more efficiently than its predecessor Fourier-Bessel steerable PCA (FBsPCA) using the non-uniform FFT. We compare the accuracy and efficiency of the new algorithm with traditional PCA and FBsPCA.

Index Terms— Cryo-electron microscopy, PCA, rotational invariance, Fourier-Bessel, non-uniform FFT

1. INTRODUCTION
Principal component analysis (PCA) is a classical method for dimensionality reduction, compression and denoising. In single particle reconstruction (SPR) using cryo-electron microscopy [1], the 3D structure of a molecule needs to be determined from many noisy 2D projection images taken at unknown viewing directions. Datasets can contain hundreds of thousands of noisy 2D projection images, with a typical image size \( 300 \times 300 \) pixels, therefore PCA is often a first step in SPR [2] to compress and denoise images. In SPR, including all planar rotations of the input images for PCA is desirable, because such images are just as likely to be obtained in the experiment, by in-plane rotating either the specimen or the detector. When all rotated images are included for PCA, the principal components have a special separation of variables form in polar coordinates in terms of radial functions and angular Fourier modes [3, 4, 5, 6, 7]. “Steering” the principal components is achieved by a simple phase shift, hence the name “steerable PCA”.

Computing the steerable PCA efficiently and accurately is however challenging. Efficient algorithms for steerable PCA were introduced in [8, 5] with computational complexity almost similar to that of traditional PCA on the original images without their rotations. However in those methods images are mapped to polar grids that do not preserve the noise statistics and yield spurious principal components that correspond to colored noise. Fourier-Bessel steerable PCA (FBsPCA) [7] combines into the steerable PCA framework a sampling criterion similar to the one introduced by Klug and Crowther [9] and represent the images in a truncated Fourier-Bessel basis using least squares. The truncated Fourier-Bessel expansion solves the problem of nonunitary transformation from Cartesian to polar grid that changes white noise to colored noise. The sampling criterion also implies that the rotationally invariant covariance matrix of the images has a block diagonal structure where the block size decreases as a function of the angular frequency. The computational complexity for FBsPCA is \( O(nL^4 + L^5) \) for \( n \) images of size \( L \times L \). Since it is more efficient than traditional PCA and gives better denoising effect [7], FBsPCA is useful in cryo-EM class averaging pipeline [10]. However, it is still too slow to analyze a large number of images of large size (i.e. large \( n \), large \( L \)). We present here a fast Fourier-Bessel steerable PCA (FFBsPCA) that reduces the computational complexity for FBsPCA by computing the Fourier-Bessel expansion coefficients more efficiently. Instead of analyzing the images in real Cartesian grid, we map the images onto polar Fourier grid using the non-uniform Fast Fourier Transform (NUFFT) [11, 12, 13]. FFBsPCA uses a sampling criterion similar to FBsPCA to truncate the Fourier-Bessel expansion. The expansion coefficients of the images are efficiently evaluated by 1D FFT on concentric rings followed by accurate evaluation of radial integral with Gaussian quadrature (GQ) rule. We take advantage of the angular fast Fourier transformation to speed up the computation so that the new algorithm can compute the steerable principal components more efficiently for large images. The overall computational complexity is reduced to \( O(nL^3 + L^4) \) which is the main contribution of this paper.

2. SAMPLING CRITERION
We assume that the set of images corresponds to objects that are essentially spatially limited in real space and bandlimited
in Fourier domain. By appropriate scaling of the pixel size or Fourier grid size, we can assume that the images vanish outside a disk of radius 1.

The eigenfunctions of the Laplacian in the unit disk with vanishing Dirichlet boundary condition are the Fourier-Bessel functions. Hence, they form an orthogonal basis to the space of squared-integrable functions over the unit disk, and it is natural to expand the images in that basis. The Fourier-Bessel functions are given by

$$\psi^{kq}(r, \theta) = \begin{cases} N_{kq}J_k(R_{kq}r)e^{ik\theta}, & r \leq 1 \\ 0, & r > 1, \end{cases} \tag{1}$$

where $N_{kq}$ is a normalization factor; $J_k$ is the Bessel function of integer order $k$; and $R_{kq}$ is the $q^{th}$ root of the Bessel function $J_k$. The functions $\psi^{kq}$ are normalized to unity, with the normalization factors $N_{kq} = \pi^{1/2}J_{k+1/2}(R_{kq})$.

We use here the following convention for the 2D Fourier transform of a function $f$ in polar coordinates

$$\mathcal{F}(f)(k_0, \phi_0) = \int_0^{2\pi} \int_0^{\infty} f(r, \theta)e^{-2\pi ik_0 r \cos(\theta - \phi_0)}r \, dr \, d\theta. \tag{2}$$

The 2D Fourier transform of the Fourier-Bessel functions, denoted $\mathcal{F}(\psi^{kq})$, is given in polar coordinates as

$$\mathcal{F}(\psi^{kq})(k_0, \phi_0) = 2\sqrt{\pi}(-1)^q(-i)^k R_{kq} \frac{J_k(2\pi k_0)}{(2\pi k_0)^2} e^{ik\phi_0}. \tag{3}$$

Notice that the Fourier transform $\mathcal{F}(\psi^{kq})(k_0, \phi_0)$ vanishes on concentric rings of radii $k_0 = \frac{R_{k(q+1)}}{2\pi}$ with $q' \neq q$. The maximum of $|\mathcal{F}(\psi^{kq})(k_0, \phi_0)|$ is obtained near the ring $k_0 = \frac{R_{kL}}{2\pi}$. For images that are sampled on a squared Cartesian grid of size $2L \times 2L$ pixels, the sampling rate is $L$ and the corresponding Nyquist frequency (the bandlimit) is $\frac{2\pi}{2L}$. For the application in the cryo-EM images, the decaying envelope of the contrast transfer function (CTF) practically implies that molecule is band limited (even below the Nyquist limit rendered by the camera). When we work with the images in the Fourier domain, we should choose a smaller cutoff $\frac{R_{kL}}{2\pi}$. The first zero after $|\mathcal{F}(\psi^{kq})|$ reaches maximum should be within the bandlimit. Due to the Nyquist criterion, the Fourier-Bessel expansion requires components for which

$$\frac{R_{k(q+1)}}{2\pi} \leq \frac{k_L}{2}, \tag{4}$$

because including other components that represent features beyond the resolution would result in aliasing. The sampling argument gives a truncation rule for Fourier-Bessel expansion, that is $R_{k(q+1)} \leq \pi k_L$.

### 3. FOURIER-BESSEL EXPANSION OF IMAGES SAMPLED ON POLAR FOURIER GRID

Suppose $I_1, \ldots, I_n$ are $n$ images sampled on a Cartesian grid. The images are resampled on a polar grid by the polar Fourier transform as in (2) using NUFFT [11][12][13]. The positions on the radial lines are not uniformly distributed. We denote by $I_i$ the continuous approximation of the Fourier transform of the $i$'th image in terms of a truncated Fourier-Bessel expansion including only components satisfying the sampling criterion, namely

$$\tilde{I}_i(r, \theta) = \sum_{k=-k_{max}}^{k_{max}} \sum_{q=1}^{p_k} a_{k,q}^{i} \psi^{kq}(r, \theta), \tag{5}$$

where for each $k$, $p_k$ denotes the number of components satisfying $R_{k(q+1)} \leq \pi k_L$, and expansion coefficients are given by

$$a_{k,q}^{i} = \int_{0}^{2\pi} \int_{0}^{1} \tilde{I}_i(r, \theta) N_{kq} J_k(R_{kq}r)e^{-ik\theta}r \, dr \, d\theta = \int_{0}^{1} N_{kq} J_k(R_{kq}r)r \, dr \int_{0}^{2\pi} \tilde{I}_i(r, \theta)e^{-ik\theta}d\theta. \tag{6}$$

We use discrete samples on a polar Fourier grid to evaluate (6). The angular integration is computed with FFT on each concentric ring and yields $I_k^L(r)$. Then the radial integration can be accurately evaluated using GQ rule [14 Chap. 4]. Specifically, we use the Gauss-Legendre quadrature rule to select $n_r$ points $\{r_j\}_{j=1}^{n_r}$ on the interval $[0, 1]$ and compute the associated weights $w(r_j)$, so that the integral is approximated by

$$a_{k,q}^{i} = \sum_{j=1}^{n_r} N_{kq} J_k(R_{kq}r_j) I_k^L(r_j)w(r_j). \tag{7}$$

In practice, we have numerically observed that oversampling on the radial lines with $n_r$ slightly larger than $k_L$ gives accurate evaluation of the integral. Although polar Fourier transformation is not a unitary transformation, representing the images with truncated Fourier-Bessel basis ensures that the transformation is almost unitary, and therefore white noise remains approximately white after the transformation.

### 4. SAMPLE COVARIANCE MATRIX

“Steering” the continuous approximation $\tilde{I}_i$ (eq. (5)) introduces a phase shift to the expansion coefficients,

$$\tilde{I}_i^\alpha(r, \theta) = \tilde{I}_i(r, \theta - \alpha) = \sum_{k,q} a_{k,q}^{i} e^{-ik\alpha} \psi^{kq}(r, \theta). \tag{8}$$

Under reflection $a_{k,q}^{i}$ changes to $a_{-k,q}^{i}$, and the reflected image, denoted $\tilde{I}_i^r$, is given by

$$\tilde{I}_i^r(r, \theta) = \tilde{I}_i(r, \pi - \theta) = \sum_{k,q} a_{-k,q}^{i} \psi^{kq}(r, \theta). \tag{9}$$

The sample mean, denoted $\tilde{I}_{\text{mean}}$, is the continuous image obtained by averaging the continuous images and all their
possible rotations and reflections:

$$
\hat{I}_{\text{mean}}(r, \theta) = \frac{1}{2n} \sum_{i=1}^{n} \frac{1}{2\pi} \int_{0}^{2\pi} \left[ \hat{I}^\alpha_i (r, \theta) + \hat{I}^{\alpha,r}_i (r, \theta) \right] \, d\alpha
$$

(10)

Substituting eqs. (8) and (9) into (10) we obtain

$$
\hat{I}_{\text{mean}}(r, \theta) = \sum_{q=1}^{p_k} \left( \frac{1}{n} \sum_{i=1}^{n} a^0_{i,q} \right) \psi^{0q}(r, \theta).
$$

(11)

As expected, the sample mean image is radially symmetric, because $\psi^{0q}$ is only a function of $r$ but not of $\theta$.

The sample covariance matrix $C$ can be directly computed from the expansion coefficients $a^k_{i,q}$. Subtracting the mean image is equivalent to subtracting the coefficients $a^0_{i,q}$ with $\frac{1}{n} \sum_{i=1}^{n} a^0_{i,q}$, while keeping other coefficients unchanged. That is, we update $a^i_{0,q} \rightarrow a^i_{0,q} - \frac{1}{n} \sum_{i=1}^{n} a^0_{i,q}$. In the Fourier-Bessel basis the covariance matrix $C$ is given by

$$
C = \frac{1}{2n} \sum_{i=1}^{n} \frac{1}{2\pi} \int_{0}^{2\pi} \left[ (\hat{I}^i - \hat{I}_{\text{mean}})(\hat{I}^i - \hat{I}_{\text{mean}})^\dagger \right. \\
\left. + (\hat{I}^{i,r} - \hat{I}_{\text{mean}})(\hat{I}^{i,r} - \hat{I}_{\text{mean}})^\dagger \right] \, d\alpha
$$

(12)

When written in terms of the Fourier-Bessel basis, the covariance matrix $C$ can be directly computed from the expansion coefficients $a^k_{i,q}$. Subtracting the mean image is equivalent to subtracting the coefficients $a^0_{i,q}$ with $\frac{1}{n} \sum_{i=1}^{n} a^0_{i,q}$, while keeping other coefficients unchanged. That is, we update $a^i_{0,q} \rightarrow a^i_{0,q} - \frac{1}{n} \sum_{i=1}^{n} a^0_{i,q}$. In the Fourier-Bessel basis the covariance matrix $C$ is given by

$$
C_{(k,q),(k',q')} = \delta_{k,k'} \frac{1}{2n} \sum_{i=1}^{n} \left( a^i_{k,q}(a^{i,*}_{k,q})^* + a^i_{-k,q}(a^{i,*}_{-k,q})^* \right),
$$

(13)

where $\delta_{k,k'}$ comes from the integral over all $\alpha$. $C$ is a block diagonal matrix because the non-zero entries of $C$ correspond to $k = k'$. Also, it suffices to consider $k \geq 0$, because $C_{(k,q),(k',q')} = C_{(-k,q),(-k',q')}$. Thus, the covariance matrix can be written as the direct sum $C = \bigoplus_{k=-\infty}^{\infty} C^{(k)}$, where $C^{(k)}_{q,q'}$ is by itself a sample covariance matrix of size $p_k \times p_k$. The block size $p_k$ decreases as the angular frequency $k$ increases. The block size must reduce as the angular frequency increases in order to avoid aliasing. Moreover, if the images are corrupted by independent additive white (uncorrelated) noise, then each block $C^{(k)}$ is also affected by approximately independent additive white noise, because the Fourier-Bessel transform is nearly unitary.

5. ALGORITHM AND COMPUTATIONAL COMPLEXITY

We refer to the resulting algorithm as Fast Fourier-Bessel steerable PCA (FFBsPCA). The steps of FFBsPCA are summarized in Algorithm 1. The computational complexity of FFBsPCA is $O(nL^3 + L^4)$, whereas the computational complexity of the traditional PCA (applied on the original images without their rotational copies) is $O(nL^4 + L^6)$ and the computational complexity of FBsPCA in [7] is $O(nL^5 + L^5)$. Therefore the new algorithm is more efficient especially for images of large size. The different steps of FFBsPCA have the following computational cost. The cost for precomputing the Bessel radial functions for all $k, q$ is $O(L^3)$, because the number of basis functions satisfying the sampling criterion is $O(L^2)$ and the number of grid points is also $O(L)$. The complexity of polar Fourier transform using NUFFT is $O(nL^2 \log \log n \log L^2)$ for $n$ images of size $2L \times 2L$. It takes $O(nL^3)$ to compute the expansion coefficients $a^k_{i,q}$ through radial integration with GQ. The computational complexity of constructing the block diagonal covariance matrix is $O(nL^3)$. Since the covariance matrix has a special block diagonal structure, its eigen-decomposition takes $O(L^4)$. Constructing the steerable basis takes $O(L^4)$. Therefore, the total computational complexity for FFBsPCA without is $O(nL^3 + L^4)$.

6. NUMERICAL EXPERIMENTS

We simulated images consisting entirely of white Gaussian noise with mean 0 and variance 1 and computed the Fourier-Bessel expansion coefficients to verify that the transformation does not change the noise statistics. The distribution of the eigenvalues for the rotational invariant covariance matrix with different angular frequencies $k$ are well predicted by the Marčenko-Pastur distribution (see Fig. 1). This shows that the transformation is nearly unitary and this property allows us to use the method described in [13] to estimate the noise variance and the number of principal components to choose for images corrupted by additive white Gaussian noise.
Fig. 1: Histogram of eigenvalues of $C^{(k)}$ for $n = 10^4$ images of size $300 \times 300$ ($L = 150$) consisting of white Gaussian noise with mean 0 and variance 1. The dashed lines correspond to the Marčenko-Pastur distribution. Cutoff in Fourier domain is $k_L = 100$.

Fig. 2: Running time for different PCA methods. (a) $n = 10^4$ and the image size $2L \times 2L$ varies and $k_L = 2/3L$. (b) The number of images varies and $L = 150$ and $k_L = 100$.

We compare the running time among FFBsPCA, FBsPCA and traditional PCA, the latter does not that does not include images’ in-plane rotations for its computation. The algorithms are implemented in MATLAB on a machine with 2 Intel(R) Xeon(R) CPUs X5570, each with 4 cores, running at 2.93 GHz. For small $L$, since FFBsPCA needs polar Fourier transformation, it appears slightly slower than the other two methods. However when $L$ increases, FFBsPCA is computationally more efficient (see Fig. 2a). We also fixed the size of the image and vary the number of images $n$. Fig. 2b shows that with $L = 150$ and $k_L = 100$, FFBsPCA is the fastest among those three methods. Timing for PCA zigzags in Fig. 2b due to the fluctuation in the efficiency of large eigendecomposition in MATLAB.

In the last experiment, we simulated $n = 10^4$ clean projection images of E. coli 70S ribosome. The images are of size $129 \times 129$ pixels. We corrupted the clean images with additive white Gaussian noise at different levels of signal-to-noise ratio (SNR) (Fig. 3) and computed steerable principal components. The top 5 principal components for noisy images agree from FFBsPCA with the principal components from clean projection images (Fig. 4a and Fig. 4d)). The principal components generated by FFBsPCA agree with those by FBsPCA and they are cleaner than the principal components from the traditional PCA (Fig. 4d, Fig. 4e and Fig. 4f)).

Fig. 3: Simulated 70S ribosome projection images with different SNR.

Fig. 4: Principal components for Fourier Transformed $10^4$ simulated 70S ribosome projection images. Clean images: (a) FFBsPCA, (b) FBsPCA and (c) traditional PCA. Noisy images with SNR = 150: (d) FFBsPCA, (e) FBsPCA and (f) traditional PCA. Image size is $129 \times 129$ pixels and $k_L = 55$.

7. CONCLUSION

We have presented a fast Fourier-Bessel steerable PCA method that reduces the computational complexity significantly with respect to the size of the images so that it can handle images of large size. This work has been mostly motivated by its application to cryo-EM. Besides compression and denoising of the experimental images, our FFBsPCA can be applied in conjunction to Kam’s approach [16] that requires the covariance matrix of the 2D images.

Finally, we remark that the Fourier-Bessel basis can be replaced in our framework with other suitable bases. For example, the 2D prolate spheroidal wave functions (PSWF) on a disk [17]. They also have a separation of variables form which makes them convenient for steerable PCA. Therefore, a similar method can be applied once the prolate radial function is numerically evaluated accurately.
8. REFERENCES


