

Direct Batch Evaluation of Optimal Orthonormal Eigenvectors of the DFT Matrix¹

Magdy Tawfik Hanna²

Abstract

The generation of Hermite-Gaussian-like orthonormal eigenvectors of the discrete Fourier transform (DFT) matrix \mathbf{F} is an essential step in the development of the discrete fractional Fourier transform (DFRFT). Most existing techniques depend on the generation of orthonormal eigenvectors of a nearly tridiagonal matrix \mathbf{S} which commutes with matrix \mathbf{F} . More sophisticated methods view the eigenvectors of \mathbf{S} as only initial ones and use them for generating final ones which better approximate the Hermite-Gaussian functions employing a technique like the orthogonal procrustes algorithm (OPA). Here a direct technique for the collective (batch) evaluation of optimal Hermite-Gaussian-like eigenvectors of matrix \mathbf{F} is contributed. It is a direct technique in the sense that it does not require the generation of initial eigenvectors to be used for computing the final superior ones. It is a batch method in the sense that it solves for the entire target modal matrix of \mathbf{F} instead of the sequential generation of the eigenvectors. The simulation results show that the proposed method is faster than the OPA.

Index Terms: DFT matrix, orthonormal eigenvectors, Hermite-Gaussian-like eigenvectors, constrained optimization, discrete fractional Fourier transform.

I. INTRODUCTION

The emergence of the discrete fractional Fourier transform (DFRFT) has revived the interest in computing orthonormal eigenvectors of the discrete Fourier transform (DFT) matrix \mathbf{F} since the orthonormality of those eigenvectors is an essential requirement for the index additivity property of the fractional transform. McClellan and Parks [1] elegantly derived the multiplicities of the eigenvalues of matrix \mathbf{F} ; however their proposed eigenvectors are not orthogonal and consequently cannot be taken as a basis for developing the DFRFT. Dickinson and Steiglitz [2] discovered a nearly tridiagonal matrix \mathbf{S} which commutes with matrix \mathbf{F} and consequently took its eigenvectors as those of \mathbf{F} . Santhanam and McClellan [3] were the first to employ the eigendecomposition of matrix \mathbf{F} for developing a definition of the DFRFT. Candan, Kutay and Ozaktas [4] discretized the second order differential equation satisfied by the Hermite-Gaussian functions – which are the eigenfunctions of the continuous fractional Fourier transform (FRFT) – and showed that one period of the periodic solution of the resulting difference equation is an eigenvector of matrix \mathbf{S} . This implies that the eigenvectors of matrix \mathbf{S} are Hermite-Gaussian-like and consequently a DFRFT defined in terms of them will approximate its continuous counterpart, namely the FRFT. Pursuing it

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² Department of Engineering Mathematics and Physics, Faculty of Engineering, Fayoum University, Fayoum 63514, Egypt, Tel: 0020-2-35706033, Fax: 0020-2-35706033, Mobile: 0108097476, Email: hanna@ieee.org

further, Pei, Yeh and Tseng [5] viewed the eigenvectors of matrix³ \mathbf{S} as only *initial* ones to be used for computing *final superior* eigenvectors in the sense of better approximating the Hermite-Gaussian functions. They employed the orthogonal procrustes algorithm (OPA) for the batch evaluation of the *final* eigenvectors. Pei et al. started their analysis by proving that vectors formed by rearranging samples of the Hermite-Gaussian functions are *approximate* eigenvectors of matrix \mathbf{F} that correspond to its *exact* eigenvalues. Actually those *approximate* eigenvectors are quite *desirable* since they are samples of the Hermite-Gaussian functions and the ultimate goal is the generation of Hermite-Gaussian-like eigenvectors. Recently Hanna, Seif and Ahmed [6] computed *initial* orthonormal eigenvectors of \mathbf{F} by the singular value decomposition (SVD) of the projection matrices of \mathbf{F} on its eigenspaces. Moreover they proved that the *final* eigenvectors of \mathbf{F} evaluated using the OPA are invariant under the change of the initial ones.

The main objective of this paper is the direct attack on the problem of deriving an *optimal* unitary modal matrix of matrix \mathbf{F} in the sense of being the closest to the matrix whose columns are formed by sampling the Hermite-Gaussian functions. More specifically the squared Frobenius norm of the difference between the target matrix and the matrix of *approximate desirable* eigenvectors will be minimized subject to the constraint that the target matrix is a unitary modal matrix of \mathbf{F} . The method is *direct* in the sense that it does not require the generation of *initial* eigenvectors as a prerequisite for computing the *final* optimal ones. The method is described as *batch* since it solves for the *entire* modal matrix of \mathbf{F} rather than *sequentially* evaluates the eigenvectors. The proposed method will be termed the *Direct Batch Evaluation by constrained Optimization Algorithm* (DBEOA).

After introducing the required mathematical notations in section II, the constrained minimization problem is solved in section III apart from evaluating two matrices \mathbf{G} and \mathbf{H} of Lagrange multipliers. Matrix \mathbf{G} is eliminated in section IV and matrix \mathbf{W} – related to matrix \mathbf{H} – is evaluated in section V. The algorithm is provided in section VI and some simulation results are presented in section VII.

II. PRELIMINARY

Although the motivation behind this work is the development of Hermite-Gaussian-like eigenvectors of the DFT matrix, the results will be presented in a more general mathematical framework where \mathbf{F} is assumed to be any unitary matrix of order N having distinct eigenvalues λ_k with algebraic multiplicities r_k , $k = 1, \dots, K$. Let E_k be the eigenspace pertaining to λ_k , i.e. the subspace of the N -dimensional complex space C^N spanned by the eigenvectors of \mathbf{F} corresponding to the eigenvalue λ_k . Since the unitarity of \mathbf{F}

³ Strictly speaking, denoting matrix \mathbf{S} in the work of Dickinson et. al. [2] and Pei et. al. [5] by \mathbf{S}_1 and matrix \mathbf{S} in the work of Candan et. al. [4] by \mathbf{S}_2 , the two matrices are related by $\mathbf{S}_2 = \mathbf{S}_1 - 4\mathbf{I}$. Therefore \mathbf{S}_1 and \mathbf{S}_2 have the same eigenvectors.

results in the orthogonality of the eigenspaces E_k , $k = 1, \dots, K$ [7], the problem of generating orthonormal eigenvectors for \mathbf{F} decouples into K separate problems where in the k^{th} problem one seeks orthonormal basis for E_k . The unitarity of \mathbf{F} implies that the geometric multiplicity of λ_k (which is the number of linearly independent eigenvectors corresponding to it) is equal to its algebraic multiplicity and consequently the dimension of E_k is r_k [8]. Let $\widehat{\mathbf{U}}_k$ be the target optimal $N \times r_k$ matrix whose columns are orthonormal basis of the eigenspace E_k and let \mathbf{U}_k be the corresponding matrix whose columns are *approximate* (since they are not exact) *but desirable* (since they have a key feature such as being samples of the Hermite-Gaussian functions) eigenvectors of \mathbf{F} pertaining to the *exact* eigenvalue λ_k . The descriptor *desirable* stems from the fact that the main goal is the generation of exact eigenvectors which are as close as possible to samples of the Hermite-Gaussian functions. It goes without saying that the columns of \mathbf{U}_k are not basis of E_k since they are *approximate* eigenvectors. It will be assumed that the columns of \mathbf{U}_k are linearly independent. The objective is to derive matrix $\widehat{\mathbf{U}}_k$ such that it is the closest matrix (in some sense) to \mathbf{U}_k .

III. BATCH EVALUATION BY CONSTRAINED OPTIMIZATION

Given matrix \mathbf{U}_k find matrix $\widehat{\mathbf{U}}_k$ that minimizes the squared Frobenius norm:

$$J_a = \left\| \mathbf{U}_k - \widehat{\mathbf{U}}_k \right\|_F^2 \quad (1)$$

subject to the constraints

$$\mathbf{A} \equiv (\mathbf{F} - \lambda_k \mathbf{I}) \widehat{\mathbf{U}}_k = \mathbf{0} \quad (2)$$

and⁴

$$\mathbf{B} \equiv \widehat{\mathbf{U}}_k^H \widehat{\mathbf{U}}_k - \mathbf{I}_{r_k} = \mathbf{0}. \quad (3)$$

Constraint (2) guarantees that the columns of $\widehat{\mathbf{U}}_k$ are eigenvectors of \mathbf{F} and constraint (3) guarantees their orthonormality. By virtue of the definition of the Frobenius norm, criterion (1) can be expressed as:

$$\begin{aligned} J_a &= \text{tr} \left[(\mathbf{U}_k - \widehat{\mathbf{U}}_k)^H (\mathbf{U}_k - \widehat{\mathbf{U}}_k) \right] \\ &= \text{tr}(\mathbf{U}_k^H \mathbf{U}_k) + \text{tr}(\widehat{\mathbf{U}}_k^H \widehat{\mathbf{U}}_k) - \text{tr}(\widehat{\mathbf{U}}_k^H \mathbf{U}_k) - \text{tr}(\mathbf{U}_k^H \widehat{\mathbf{U}}_k) \\ &= \text{tr}(\mathbf{U}_k^H \mathbf{U}_k) + r_k - 2 \text{Real} \{ \text{tr}(\widehat{\mathbf{U}}_k^H \mathbf{U}_k) \} \end{aligned} \quad (4)$$

where $\text{tr}(\cdot)$ is the trace of a matrix and $\text{Real}\{\cdot\}$ denotes the real part. The above equation implies that minimizing J_a w.r.t. $\widehat{\mathbf{U}}_k$ is equivalent to maximizing the following criterion:

⁴ The superscripts ^T, ^{*}, ^H respectively denote the transpose, the complex conjugate and the Hermitian transpose (i.e. the complex conjugate transpose).

$$J_b = tr(\widehat{\mathbf{U}}_k^H \mathbf{U}_k) + tr(\mathbf{U}_k^H \widehat{\mathbf{U}}_k). \quad (5)$$

Augmenting this real criterion by the two sets of constraints (2) and (3), one gets the following real augmented maximization criterion:

$$J = J_b - \boldsymbol{\mu}^T (\mathbf{G}^* \circ \mathbf{A}) \boldsymbol{\mu} - \boldsymbol{\mu}^T (\mathbf{G} \circ \mathbf{A}^*) \boldsymbol{\mu} - \boldsymbol{\mu}^T (\mathbf{H}^* \circ \mathbf{B}) \boldsymbol{\mu} - \boldsymbol{\mu}^T (\mathbf{H} \circ \mathbf{B}^*) \boldsymbol{\mu} \quad (6)$$

where \mathbf{G} and \mathbf{H} are matrices of Lagrange multipliers, the symbol \circ denotes the Schur product of matrices (see its definition in [9, Appendix]), and $\boldsymbol{\mu}$ is the summing vector defined by

$$\boldsymbol{\mu} = (1 \ 1 \ \dots \ 1)^T. \quad (7)$$

Using (2) and (7), one gets

$$\boldsymbol{\mu}^T (\mathbf{G}^* \circ \mathbf{A}) \boldsymbol{\mu} = \sum_{j=1}^{r_k} \sum_{i=1}^N g_{ij}^* a_{ij} = \sum_{j=1}^{r_k} \mathbf{g}_j^H \mathbf{a}_j = \sum_{j=1}^{r_k} \mathbf{g}_j^H (\mathbf{F} - \lambda_k \mathbf{I}) \widehat{\mathbf{u}}_j \quad (8)$$

where \mathbf{g}_j and \mathbf{a}_j are respectively the j th column of the matrices \mathbf{G} and \mathbf{A} . Using (3) and (7), one gets:

$$\boldsymbol{\mu}^T (\mathbf{H}^* \circ \mathbf{B}) \boldsymbol{\mu} = \sum_{j=1}^{r_k} \sum_{i=1}^{r_k} h_{ij}^* b_{ij} = \sum_{j=1}^{r_k} \sum_{i=1}^{r_k} h_{ij}^* (\widehat{\mathbf{u}}_i^H \widehat{\mathbf{u}}_j - \delta_{ij}) \quad (9)$$

where δ_{ij} is the Kronecker delta. Substituting (5), (8) and (9) in (6), one gets

$$\begin{aligned} J = & \sum_{i=1}^{r_k} \widehat{\mathbf{u}}_i^H \mathbf{u}_i + \sum_{i=1}^{r_k} \mathbf{u}_i^H \widehat{\mathbf{u}}_i - \sum_{j=1}^{r_k} \mathbf{g}_j^H (\mathbf{F} - \lambda_k \mathbf{I}) \widehat{\mathbf{u}}_j - \sum_{j=1}^{r_k} \widehat{\mathbf{u}}_j^H (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{g}_j \\ & - \sum_{j=1}^{r_k} \sum_{i=1}^{r_k} h_{ij}^* (\widehat{\mathbf{u}}_i^H \widehat{\mathbf{u}}_j - \delta_{ij}) - \sum_{j=1}^{r_k} \sum_{i=1}^{r_k} h_{ij} (\widehat{\mathbf{u}}_j^H \widehat{\mathbf{u}}_i - \delta_{ij}) \end{aligned} \quad (10)$$

The necessary conditions for the maximization of J are:

$$\nabla_{\widehat{\mathbf{u}}_m} J = \mathbf{0} \quad , m = 1, \dots, r_k \quad (11)$$

$$\nabla_{\mathbf{g}_m} J = \mathbf{0} \quad , m = 1, \dots, r_k \quad (12)$$

$$\nabla_{h_{ij}} J = 0 \quad , i = 1, \dots, r_k \quad , \quad j = 1, \dots, r_k \quad (13)$$

In evaluating the gradient vector w.r.t. $\widehat{\mathbf{u}}_m$ in (11) one should view $\widehat{\mathbf{u}}_m$ and $\widehat{\mathbf{u}}_m^*$ as two different vectors, i.e. one should treat $\widehat{\mathbf{u}}_m$ as a constant vector when finding $\nabla_{\widehat{\mathbf{u}}_m}$ [10]. The same remark applies to the gradients in (12) and (13). One should notice that conditions (12) and (13) lead to the constraints (2) and (3) respectively. In preparation for applying the remaining condition (11), one takes the gradient of (10) to get

$$\begin{aligned} \nabla_{\widehat{\mathbf{u}}_m} J = & \mathbf{u}_m - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{g}_m - \sum_{j=1}^{r_k} h_{mj}^* \widehat{\mathbf{u}}_j - \sum_{i=1}^{r_k} h_{im} \widehat{\mathbf{u}}_i \\ = & \mathbf{u}_m - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{g}_m - \sum_{i=1}^{r_k} (h_{im} + h_{mi}^*) \widehat{\mathbf{u}}_i \\ = & \mathbf{u}_m - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{g}_m - \widehat{\mathbf{U}}_k \left[\mathbf{h}_m + (\mathbf{h}^{(m)})^H \right] \end{aligned} \quad (14)$$

where \mathbf{h}_m and $\mathbf{h}^{(m)}$ are respectively the m th column and row of matrix \mathbf{H} and

$$\hat{\mathbf{U}}_k = (\hat{\mathbf{u}}_1 \quad \hat{\mathbf{u}}_2 \quad \cdots \quad \hat{\mathbf{u}}_{r_k}). \quad (15)$$

Applying the set of conditions (11) to (14), one gets

$$\hat{\mathbf{U}}_k [\mathbf{h}_m + (\mathbf{h}^{(m)})^H] = \mathbf{u}_m - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{g}_m, \quad m = 1, \dots, r_k. \quad (16)$$

This set of r_k vector equations can be compactly expressed as one matrix equation

$$\hat{\mathbf{U}}_k (\mathbf{H} + \mathbf{H}^H) = \mathbf{U}_k - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{G} \quad (17)$$

where

$$\mathbf{U}_k = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_{r_k}). \quad (18)$$

Equation (17) can be expressed as

$$\hat{\mathbf{U}}_k \mathbf{W} = \mathbf{U}_k - (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{G} \quad (19)$$

where \mathbf{W} is the Hermitian matrix of order r_k defined by

$$\mathbf{W} = \mathbf{H} + \mathbf{H}^H. \quad (20)$$

In order to arrive at the target matrix $\hat{\mathbf{U}}_k$ it remains to find the two matrices \mathbf{G} and \mathbf{W} and eliminate them from (19).

IV. ELIMINATION OF LAGRANGE MULTIPLIERS MATRIX \mathbf{G}

Matrix \mathbf{G} will be eliminated by applying the first set of constraints expressed by (2). Premultiplying (19) by $(\mathbf{F} - \lambda_k \mathbf{I})$ and applying (2), one gets

$$(\mathbf{F} - \lambda_k \mathbf{I})(\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{G} = (\mathbf{F} - \lambda_k \mathbf{I})\mathbf{U}_k. \quad (21)$$

Since matrix \mathbf{F} is unitary, it is diagonalizable [8]; moreover its modal matrix can be taken to be unitary. Therefore a modal decomposition of \mathbf{F} is given by

$$\mathbf{F} = \mathbf{V}\mathbf{D}\mathbf{V}^H \quad (22)$$

where \mathbf{V} is a unitary modal matrix and \mathbf{D} is a diagonal matrix. It follows that

$$\mathbf{F} - \lambda_k \mathbf{I} = \mathbf{V}(\mathbf{D} - \lambda_k \mathbf{I})\mathbf{V}^H. \quad (23)$$

Upon substituting (23) in (21), one gets

$$\mathbf{V}(\mathbf{D} - \lambda_k \mathbf{I})(\mathbf{D} - \lambda_k \mathbf{I})^H \mathbf{V}^H \mathbf{G} = \mathbf{V}(\mathbf{D} - \lambda_k \mathbf{I})\mathbf{V}^H \mathbf{U}_k. \quad (24)$$

Let K be the number of distinct eigenvalues of \mathbf{F} which implies that matrix \mathbf{D} can be expressed as

$$\mathbf{D} = \text{Diag}\{\lambda_1 \mathbf{I}, \lambda_2 \mathbf{I}, \dots, \lambda_K \mathbf{I}\}. \quad (25)$$

The corresponding partitioned form of \mathbf{V} is

$$\mathbf{V} = (\mathbf{V}_1 \quad \mathbf{V}_2 \quad \cdots \quad \mathbf{V}_K). \quad (26)$$

Premultiplying both sides of (24) by \mathbf{V}^{-1} and utilizing (25) and (26), equation (24) reduces to the following set of K matrix equations⁵

$$|\lambda_i - \lambda_k|^2 \mathbf{V}_i^H \mathbf{G} = (\lambda_i - \lambda_k) \mathbf{V}_i^H \mathbf{U}_k \quad , i = 1, \dots, K. \quad (27)$$

For $i = k$, the above equation is immediately satisfied. Therefore \mathbf{G} should be chosen to satisfy the following $(K - 1)$ matrix equations:

$$(\lambda_i - \lambda_k)^* \mathbf{V}_i^H \mathbf{G} = \mathbf{V}_i^H \mathbf{U}_k \quad , i = 1, \dots, K \quad , \quad i \neq k. \quad (28)$$

Using (23), (25), (26) and (28), one obtains

$$\begin{aligned} (\mathbf{F} - \lambda_k \mathbf{I})^H \mathbf{G} &= \mathbf{V} (\mathbf{D} - \lambda_k \mathbf{I})^H \mathbf{V}^H \mathbf{G} \\ &= \sum_{\substack{i=1 \\ i \neq k}}^K \mathbf{V}_i (\lambda_i - \lambda_k)^* \mathbf{V}_i^H \mathbf{G} \\ &= \sum_{\substack{i=1 \\ i \neq k}}^K \mathbf{V}_i \mathbf{V}_i^H \mathbf{U}_k \end{aligned} \quad (29)$$

The unitarity of \mathbf{V} together with (26) lead to

$$\mathbf{I} = \mathbf{V} \mathbf{V}^H = \sum_{i=1}^K \mathbf{V}_i \mathbf{V}_i^H. \quad (30)$$

This implies that

$$\sum_{\substack{i=1 \\ i \neq k}}^K \mathbf{V}_i \mathbf{V}_i^H = \mathbf{I} - \mathbf{P}_k \quad (31)$$

where \mathbf{P}_k is the orthogonal projection matrix on the k^{th} eigenspace of \mathbf{F} and is given by

$$\mathbf{P}_k = \mathbf{V}_k \mathbf{V}_k^H. \quad (32)$$

Therefore matrix \mathbf{G} can be eliminated from (19) by using (29) and (31) resulting in

$$\hat{\mathbf{U}}_k \mathbf{W} = \mathbf{P}_k \mathbf{U}_k. \quad (33)$$

V. EVALUATION OF MATRIX \mathbf{W} AND SOLUTION FOR MATRIX $\hat{\mathbf{U}}_k$

(A) Evaluation of matrix \mathbf{W}

The Hermitian matrix \mathbf{W} will be determined using the second set of constraints expressed by (3). One starts by using (33) in order to get

⁵ Since the k^{th} eigenspace E_k is under consideration, the subscript k is fixed.

$$\mathbf{W}^H \widehat{\mathbf{U}}_k^H \widehat{\mathbf{U}}_k \mathbf{W} = \mathbf{U}_k^H \mathbf{P}_k^H \mathbf{P}_k \mathbf{U}_k. \quad (34)$$

Since \mathbf{P}_k is a projection matrix, it satisfies

$$\mathbf{P}_k^H = \mathbf{P}_k \quad \text{and} \quad \mathbf{P}_k^2 = \mathbf{P}_k. \quad (35)$$

Applying condition (3) together with the above condition one finds that (34) reduces to

$$\mathbf{W}^2 = \mathbf{W}^H \mathbf{W} = \mathbf{U}_k^H \mathbf{P}_k^H \mathbf{P}_k \mathbf{U}_k = \mathbf{U}_k^H \mathbf{P}_k \mathbf{U}_k. \quad (36)$$

The above equation can be expressed as

$$\mathbf{W}^2 = \widetilde{\mathbf{U}}_k^H \widetilde{\mathbf{U}}_k \quad (37)$$

where

$$\widetilde{\mathbf{U}}_k \equiv \mathbf{P}_k \mathbf{U}_k. \quad (38)$$

This implies that the columns of $\widetilde{\mathbf{U}}_k$ are the orthogonal projection of the corresponding columns of \mathbf{U}_k on the k^{th} eigenspace of matrix \mathbf{F} . It will be assumed that the columns of $\widetilde{\mathbf{U}}_k$ are linearly independent which results in the nonsingularity of \mathbf{W}^2 based on the form of (37). Consequently the Hermitian matrix \mathbf{W}^2 is positive definite and its singular value decomposition is given by

$$\mathbf{W}^2 = \mathbf{T} \mathbf{\Lambda} \mathbf{T}^H \quad (39)$$

where \mathbf{T} is a unitary matrix and

$$\mathbf{\Lambda} = \text{Diag}\{d_1, \dots, d_{r_k}\} \quad (40)$$

with $d_1 \geq d_2 \geq \dots \geq d_{r_k} > 0$. Although (39) can also be regarded as an eigenvalue decomposition of \mathbf{W}^2 , one should never try to apply a general purpose eigendecomposition routine to implement the decomposition because \mathbf{W}^2 might have repeated eigenvalues and the corresponding eigenvectors may not be orthogonal. Utilizing a singular value decomposition (SVD) routine will guarantee the unitarity of matrix \mathbf{T} in (39). The square root of \mathbf{W}^2 can generally be expressed as

$$\mathbf{W} = \mathbf{T} \mathbf{S} \mathbf{T}^H \quad (41)$$

where

$$\mathbf{S} = \text{Diag}\{\pm \sqrt{d_1}, \dots, \pm \sqrt{d_{r_k}}\}. \quad (42)$$

(B) Solving for Matrix $\widehat{\mathbf{U}}_k$

Having determined \mathbf{W} (apart of the signs of the diagonal elements of \mathbf{S}), the solution of (33) is obtained as

$$\widehat{\mathbf{U}}_k = \mathbf{P}_k \mathbf{U}_k \mathbf{W}^{-1} \quad (43)$$

where \mathbf{W}^{-1} is determined from (41) as

$$\mathbf{W}^{-1} = \mathbf{T}\mathbf{S}^{-1}\mathbf{T}^H. \quad (44)$$

In the final expression of $\hat{\mathbf{U}}_k$ given by (43), the presence of the premultiplying projection matrix \mathbf{P}_k guarantees that the columns of $\hat{\mathbf{U}}_k$ are eigenvectors of \mathbf{F} pertaining to the k^{th} eigenspace; hence constraint (2) is satisfied. It is straightforward to show that (43) satisfies constraint (3). It remains to select the single matrix out of the 2^{r_k} matrices given by (42) which maximizes criterion (5). Using (43), (35) and (36) one gets

$$\hat{\mathbf{U}}_k^H \mathbf{U}_k = \mathbf{W}^{-H} \mathbf{U}_k^H \mathbf{P}_k^H \mathbf{U}_k = \mathbf{W}^{-1} \mathbf{W}^2 = \mathbf{W}. \quad (45)$$

The above equation together with (41) and the properties of the trace of a matrix lead to

$$\text{tr}(\hat{\mathbf{U}}_k^H \mathbf{U}_k) = \text{tr}(\mathbf{T}\mathbf{S}\mathbf{T}^H) = \text{tr}(\mathbf{T}^H \mathbf{T}\mathbf{S}) = \text{tr}(\mathbf{S}). \quad (46)$$

The last equation together with (42) and (5) result in

$$J_b = 2 \sum_{i=1}^{r_k} (\pm \sqrt{d_i}) \quad (47)$$

Therefore the criterion J_b is maximized when all the signs on the R.H.S. of the above equation are positive.

Consequently matrix \mathbf{S} in (42) is uniquely determined as

$$\mathbf{S} = \text{Diag}\{\sqrt{d_1}, \dots, \sqrt{d_{r_k}}\}. \quad (48)$$

VI. THE ALGORITHM

Based on the theoretical findings of last section the *direct batch evaluation by constrained optimization algorithm* (DBEOA) can be summarized in the following steps:

1. Form matrix \mathbf{W}^2 as $\mathbf{W}^2 = \mathbf{U}_k^H (\mathbf{P}_k \mathbf{U}_k)$.
2. Find the SVD of \mathbf{W}^2 as $\mathbf{W}^2 = \mathbf{T}\mathbf{\Lambda}\mathbf{T}^H$.
3. Compute \mathbf{W}^{-1} as $\mathbf{W}^{-1} = \mathbf{T}\mathbf{S}^{-1}\mathbf{T}^H$ where \mathbf{S} is given by (48) and (40).
4. Evaluate $\hat{\mathbf{U}}_k$ as $\hat{\mathbf{U}}_k = (\mathbf{P}_k \mathbf{U}_k) \mathbf{W}^{-1}$.

The computational load of finding the optimal basis of the k^{th} eigenspace consists mainly of one SVD of a square Hermitian matrix of order r_k and four matrix multiplications. The SVD requires⁶ $O(r_k^3)$ floating

⁶ The symbol $O(\dots)$ stands for the order of magnitude.

point operations (flops) where an operation stands for a multiplication and an addition [11] and the four matrix multiplications require $r_k(N^2 + 2Nr_k + r_k^2)$ flops.

In the orthogonal procrustes algorithm (OPA) expounded in [12] and used in [5] and [6], one seeks the minimization of criterion (1) with the desired matrix $\hat{\mathbf{U}}_k$ expressed as

$$\hat{\mathbf{U}}_k = \mathbf{V}_k \mathbf{Q}_k \quad (49)$$

where \mathbf{V}_k is assumed to be a known $N \times r_k$ matrix whose columns form an *initial* orthonormal basis of the eigenspace E_k and \mathbf{Q}_k is a unitary matrix to be solved for by the algorithm. The form (49) ensures that the columns of $\hat{\mathbf{U}}_k$ are eigenvectors of \mathbf{F} and hence (49) is equivalent to constraint (2). The unitarity condition on \mathbf{Q}_k ensures the orthonormality of the columns of $\hat{\mathbf{U}}_k$ and hence it is equivalent to constraint (3). Consequently the DBEOA and OPA are two solutions of the same constrained optimization problem and should produce identical results if there is no round off error involved in the lengthy computation; which will never be the case. Stated another way, there might be some discrepancy between the outputs of the DBEOA and OPA because they are algorithmically quite distinct despite being theoretically equivalent.

Apart from the prerequisite of generating initial orthonormal eigenvectors of \mathbf{F} , one needs to perform – for each eigenspace – one SVD of a square matrix of order r_k and three matrix multiplications in order to implement the OPA. The SVD requires $O(r_k^3)$ flops and the three matrix multiplications require $r_k^2(2N + r_k)$ flops. In the case of the DFT matrix and if one employed the technique contributed by Candan et al. [4] for generating the *initial* eigenvectors by the eigendecomposition of the nearly tridiagonal matrix \mathbf{S} proposed by Dickinson and Steiglitz [2], one has to first generate matrix \mathbf{S} and perform two matrix multiplications each requiring N^3 flops in order to single out two real symmetric tridiagonal matrices each of order $q \approx 0.5N$. Next eigendecomposition is applied to each of these two matrices which requires $O(q^3)$ flops [13]. This implies that the DBEOA is definitely more computationally efficient than the OPA.

VII. SIMULATION RESULTS

The general results of this paper are applied to the DFT matrix where the number of eigenspaces is $K = 4$ and where the columns of the matrices $\mathbf{U}_k, k = 1, \dots, 4$ are rearranged samples of the Hermite-Gaussian functions [5]. The optimal eigenvectors, i.e. the matrices $\hat{\mathbf{U}}_k, k = 1, \dots, 4$ are computed using both the DBEOA of section VI and the OPA where in the latter case the required initial eigenvectors (i.e. the four matrices $\mathbf{V}_k, k = 1, \dots, 4$ mentioned in (49)) are generated by the eigendecomposition of the nearly tridiagonal matrix \mathbf{S} [4]. For each of the DBEOA and OPA the Euclidean norm of the error vectors between

the *optimal* eigenvectors (the columns of the matrices $\hat{\mathbf{U}}_k, k=1, \dots, 4$) and the *approximate but desirable* eigenvectors (the columns of the matrices $\mathbf{U}_k, k=1, \dots, 4$) are computed and plotted.

In the absence of round off error – which is unavoidable in floating point computation – the two techniques DBEOA and OPA would produce identical results. It has been found by simulation that there is no noticeable difference in their outputs for values of N up to 256. However for higher values of N some discrepancy in the norms of the error vectors $\mathbf{e}_m \equiv (\hat{\mathbf{u}}_m - \mathbf{u}_m), m=1, \dots, N$ for large values of m becomes obvious. Figure 1 shows the norms of the error vectors for both techniques for $N=512$. Table 1 depicts the computation time (in seconds) of the final eigenvectors given the approximate ones. The conclusion is that the DBEOA is faster than the OPA. In order to check the *numerical* orthonormality of the optimal eigenvectors, the *orthonormality error matrix* $(\hat{\mathbf{U}}^H \hat{\mathbf{U}} - \mathbf{I})$ - which is theoretically zero – is computed. Two measures of the orthonormality error – namely the maximum element in absolute value of this matrix as well as its Frobenius norm – are computed and given in Table 2. One notices that the orthonormality error is negligible for both the DBEOA and OPA for values of N as large as 256 which is regarded as a large value given that both methods are sophisticated and involve SVD of matrices of order $r_k \approx 0.25N$. Although the OPA seems to have a better numerical robustness, one should observe that the orthonormality error in the DBEOA case does not always grow steadily with N since its value for $N=2000$ is less than its value for $N=1024$.

Only for the sake of comparison the results of the Gram-Schmidt Algorithm (GSA) – which is based on a completely different rationale [5] – are also given in Fig. 1 and Tables 1 and 2. Figure 1 shows that for all methods the norms of the error vectors become relatively large for large values of m ($m > 0.5N$). The interpretation is that for large m , samples of the Hermite-Gaussian function of order m become a poorly approximate eigenvector of the DFT matrix as was proved in [5]. The general observation is that the GSA has a larger error for values of m close to N compared to both the OPA and DBEOA; however it has the merit that the threshold value of m where the error becomes noticeable is larger. An examination of Table 2 shows that the GSA seems to be less numerically robust than both the OPA and DBEOA.

VIII. CONCLUSION

The evaluation of optimal orthonormal eigenvectors of the DFT matrix \mathbf{F} in the sense of being the closest to *approximate* eigenvectors – formed by samples of the Hermite Gaussian functions - is formulated as a constrained optimization problem where the minimization criterion is the squared Frobenius norm of the difference between the matrices of the exact and approximate eigenvectors. The method is direct in the sense of not requiring prior generation of initial exact eigenvectors. The unitarity of matrix \mathbf{F} is exploited in

decoupling the problem such that optimal orthonormal basis for each individual eigenspace are batch evaluated. The contributed *direct batch evaluation by constrained optimization algorithm* (DBEOA) has been shown by both analysis and simulation to be faster than the orthogonal procrustes algorithm (OPA).

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Table 1: The computation time (in seconds)

N	OPA	DBEOA	GSA
32	0.0625	0.03125	0.015625
128	0.078125	0.03125	0.0625
256	0.375	0.171875	0.421875
512	2.96875	1.1875	3.390625
1024	22.96875	8.265625	27.359375
2000	191.0625	57.71875	220.3125

Table 2: Two measures of the orthonormality error

N	OPA		DBEOA		GSA	
	Maximum	Frobenius norm	Maximum	Frobenius norm	Maximum	Frobenius norm
32	2.78E-15	8.25223E-15	2E-15	1.40816E-14	7.68E-16	4.07316E-15
128	4E-15	2.8328E-14	4.85E-10	1.99582E-09	5.56E-12	8.54883E-12
256	3.33E-15	5.19285E-14	0.00778	0.043024189	0.914656	1.3346918
512	6.66E-15	9.77425E-14	0.269404	4.1853546	0.999647	18.772675
1024	6E-15	1.99409E-13	0.733461	16.833423	0.996978	49.52763
2000	2.6E-14	4.02989E-13	0.354972	14.061739	0.998109	144.06594

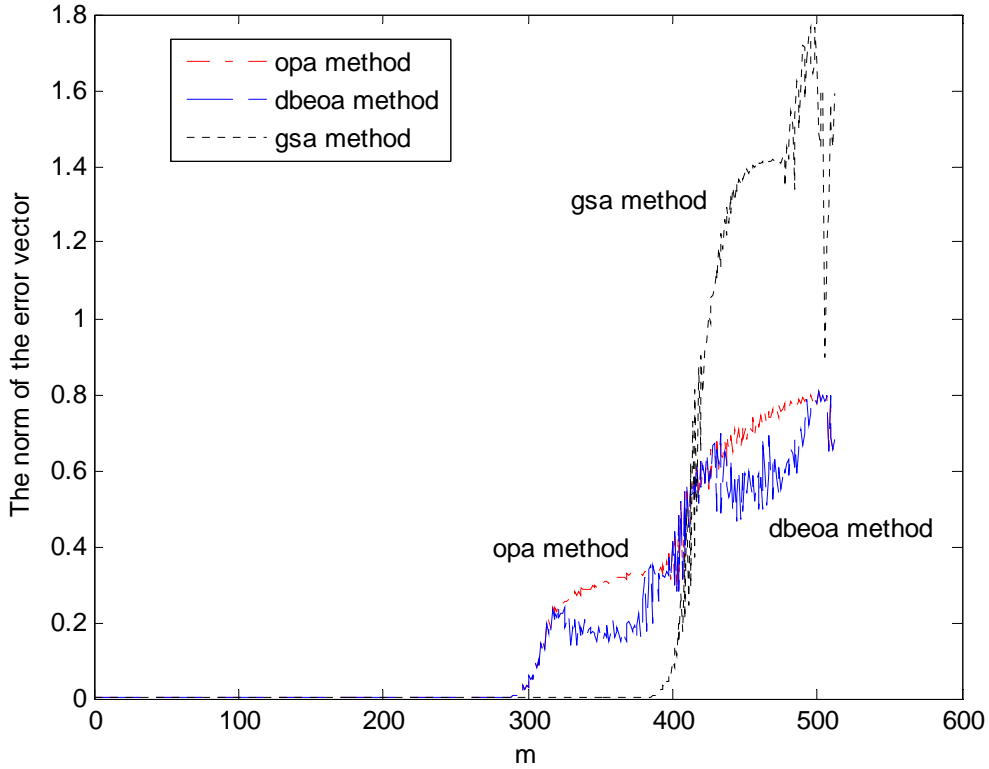


Fig. 1: The norm of the error vectors $\mathbf{e}_m \equiv (\hat{\mathbf{u}}_m - \mathbf{u}_m)$, $m = 1, \dots, N$ between the exact and approximate eigenvectors for $N = 512$.