

Direct Sequential Evaluation of Optimal Orthonormal Eigenvectors of the Discrete Fourier Transform Matrix by Constrained Optimization

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ABSTRACT

The recent emergence of the discrete fractional Fourier transform has spurred research activity aiming at generating Hermite-Gaussian-like (HGL) orthonormal eigenvectors of the discrete Fourier transform (DFT) matrix \mathbf{F} . By exploiting the unitarity of matrix \mathbf{F} – resulting in the orthogonality of its eigenspaces pertaining to the distinct eigenvalues – the problem decouples into finding orthonormal eigenvectors for each eigenspace separately. A Direct Sequential Evaluation by constrained Optimization Algorithm (DSEOA) is contributed for the generation of optimal orthonormal eigenvectors for each eigenspace separately. This technique is *direct* in the sense that it does not require the generation of initial orthonormal eigenvectors as a prerequisite for obtaining the final optimal ones. The resulting eigenvectors are *optimal* in the sense of being as close as possible to samples of the Hermite-Gaussian functions. The technique is found to be numerically robust because total pivoting is allowed in performing the QR matrix decomposition step. The DSEOA is proved to be theoretically equivalent to each of the *Gram-Schmidt algorithm* (GSA) and the *sequential orthogonal procrustes algorithm* (SOPA). However the three techniques are algorithmically quite distinct. An extensive comparative simulation study shows that the DSEOA is by far the most numerically robust technique among all sequential algorithms thus paying off for its relatively long computation time.

Indexing Terms: DFT matrix, discrete fractional Fourier transform (DFRFT), Gram-Schmidt algorithm (GSA), QR matrix decomposition, orthonormal Hermite-Gaussian-like (HGL) eigenvectors.

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1. Introduction

The revived research activity in the computation of orthonormal eigenvectors of the discrete Fourier transform (DFT) matrix \mathbf{F} is due to the emergence of the discrete fractional Fourier transform (DFRFT) [1]. The desired index additivity property of the DFRFT necessitates the orthonormality of the eigenvectors of matrix \mathbf{F} . Although McClellan and Parks developed an analytical method for generating a complete set of eigenvectors [2], this set cannot be taken as a basis for defining the DFRFT due to its lack of orthogonality. The eigenvectors of the real symmetric nearly tridiagonal matrix \mathbf{S} – discovered by Dickinson and Steiglitz [3] – which commutes with matrix \mathbf{F} are guaranteed to be orthogonal and to be eigenvectors of \mathbf{F} whenever the eigenvalues of \mathbf{S} are simple. However in the degenerate case when \mathbf{S} has an eigenvalue of multiplicity two, the two corresponding eigenvectors – evaluated by applying a general eigenanalysis software routine – will generally neither be orthogonal nor be eigenvectors of \mathbf{F} . Candan, Kutay and Ozaktas [4] have the credit of arriving at a similarity transformation reducing matrix \mathbf{S} to a block diagonal form and of developing an algorithm for generating an orthogonal set of eigenvectors common to both the \mathbf{S} and \mathbf{F} matrices irrespective of the multiplicities of the eigenvalues of \mathbf{S} . Their work has been put on a more rigorous mathematical foundation by Hanna, Seif and Ahmed [5]. Moreover Candan et al. proved that the eigenvectors of \mathbf{S} are solutions of the difference equation resulting from discretizing the differential equation satisfied by the Hermite-Gaussian functions. Consequently a DFRFT defined in terms of those Hermite-Gaussian-like (HGL) eigenvectors will approximate its continuous-time counterpart; namely the *FRactional Fourier Transform* (FRFT) since the Hermite-Gaussian functions are the eigenfunctions of both the classical Fourier transform and the FRFT [6].

Pursuing it further, Pei, Yeh and Tseng [7] looked at the eigenvectors of \mathbf{S} as only *initial* eigenvectors of \mathbf{F} and looked for *final* superior ones in the sense of better approximating vectors formed by rearranged samples of the Hermite-Gaussian functions and proved that the latter vectors are approximate eigenvectors of \mathbf{F} . They used two techniques based on different rationales for generating the *final* eigenvectors for each eigenspace individually. In the first technique termed the *Gram-Schmidt algorithm* (GSA), the approximate eigenvectors pertaining to one eigenvalue are projected on the corresponding eigenspace spanned by the *initial* exact eigenvectors pertaining to that eigenvalue and are next orthonormalized by the Gram-Schmidt procedure. In the second technique the *final* eigenvectors pertaining to one eigenspace are *batch* evaluated using the *orthogonal procrustes algorithm* (OPA) where the Frobenius norm of the difference between the matrices of the *final exact* eigenvectors and the approximate ones is minimized. In a completely independent endeavor, Pei, Tseng and Yeh [8] generated a complete set of N orthonormal HGL eigenvectors of matrix \mathbf{F} of order N by solving a series of N constrained optimization problems using the Lagrange multipliers technique without exploiting the orthogonality of the eigenspaces of matrix \mathbf{F} resulting from its unitarity. Recently Pei, Hsue and Ding [9] arrived at another nearly tridiagonal matrix - which commutes with matrix \mathbf{F} - whose eigenvectors are more HGL than those of matrix \mathbf{S} used in [3,4,5,7].

Along a different line of development, Hanna, Seif and Ahmed [10] generated *initial* orthonormal eigenvectors of \mathbf{F} by the singular value decomposition of its orthogonal projection matrices on its eigenspaces. They contributed the *sequential orthogonal procrustes algorithm* (SOPA) as a third approach – in addition to the GSA and OPA – for generating *final* superior eigenvectors given *initial* ones. Moreover they proved that the final eigenvectors – evaluated using the GSA, OPA or SOPA – are invariant under the change of the initial ones. Recently they showed that the GSA, OPA and SOPA can be applied for

generating the final superior eigenvectors – without having to first generate initial ones – by the direct utilization of the orthogonal projection matrices on the eigenspaces of matrix \mathbf{F} [11]. More recently Hanna contributed the *Direct Batch Evaluation by constrained Optimization Algorithm* (DBEOA) for the *batch* generation of optimal orthonormal eigenvectors of matrix \mathbf{F} by solving one constrained optimization problem for each eigenspace [12]. Although the DBEOA and OPA are theoretically equivalent, they are algorithmically quite distinct. The DBEOA has been shown to be faster than the OPA. A survey of the state of the art in the development of the discrete fractional Fourier transform using various approaches including the eigendecomposition of the DFT matrix \mathbf{F} can be found in [13].

In contrast to [12] which deals with the *batch* generation of optimal eigenvectors, the present paper concentrates on the *sequential* generation. More specifically a numerically stable and computationally efficient *Direct Sequential Evaluation by constrained Optimization Algorithm* (DSEOA) will be developed where the orthogonality of the eigenspaces of matrix \mathbf{F} is exploited in reducing the computational load and where total pivoting in performing the QR matrix decomposition is employed in order to improve the accuracy of the computation. It will be rigorously proved that the three sequential algorithms – namely the DSEOA, GSA and SOPA – are theoretically equivalent despite being algorithmically quite distinct. This implies that in the absence of the round off error – which is unavoidable – the three algorithms should produce identical results. Simulation results will show that for a large order of matrix \mathbf{F} , the DSEOA is by far more numerically robust than the GSA and SOPA.

The main theoretical contributions of the present paper – as compared to [8] – are the exploitation of the orthogonality of the eigenspaces of matrix \mathbf{F} in generating the eigenvectors pertaining to distinct eigenvalues separately, the adoption of complex formalism

instead of splitting the constraints into their real and imaginary parts with the purpose of reducing the number of constraints, and the selection of the total pivoting option in performing the QR matrix decomposition with a definite improvement in the accuracy of the computation. Another contribution is the proof of the theoretical equivalence of the DSEOA and GSA. First it should be emphasized that the derivation leading to the DSEOA is completely different than that leading to the GSA proposed in [7]. Second the algorithmic details of the DSEOA and GSA are quite distinct; consequently the performance of both algorithms for large values of the order N of the DFT matrix is definitely different as will be testified by the simulation results. It is obvious that the DSEOA is not at all an interpretation of the GSA. It should be pointed out that the GSA advocated in [7] and the constrained eigendecomposition of the DFT matrix by Lagrange multiplier method promulgated in [8] have existed as isolated islands; the fact that they are theoretically equivalent is being brought to light for the first time here.

The main practical finding of the present work is that the contributed DSEOA is the most numerically accurate *sequential* technique for generating HGL orthonormal eigenvectors of the DFT matrix \mathbf{F} . Since the DFRFT depends heavily on having those target eigenvectors, the contributed technique helps advance the state of the art in the development of the DFRFT. Actually the quest of the signal processing and optics communities for having excellent HGL eigenvectors of matrix \mathbf{F} is not expected to end.

After laying out the mathematical framework in section 2, the DSEOA is developed in section 3. The theoretical equivalence of the DSEOA and GSA is proved in section 4. An extensive comparative simulation study is carried out in section 5.

2. A Mathematical Framework

For the sake of generality the DSEOA reported next section - as well as the GSA and SOPA - apply to any unitary matrix \mathbf{F} of order N rather than being confined to the DFT matrix. Let the distinct eigenvalues of \mathbf{F} be λ_k with algebraic multiplicities r_k , $k = 1, \dots, K$. Let E_k be the eigenspace corresponding to λ_k , i.e. the subspace of the N -dimensional complex space C^N spanned by the eigenvectors of \mathbf{F} pertaining to λ_k . The unitarity of \mathbf{F} implies the orthogonality of the eigenspaces E_k , $k = 1, \dots, K$ [14]. Consequently the problem of generating orthonormal eigenvectors of \mathbf{F} can be decoupled into K separate problems where in the k^{th} problem one seeks desired orthonormal basis for E_k . The unitarity of \mathbf{F} also implies that the geometric multiplicity of λ_k (which is the number of linearly independent eigenvectors pertaining to it) is equal to its algebraic multiplicity and consequently the dimension of E_k is r_k [15]. Let \mathbf{U}_k be a matrix whose columns are *approximate* eigenvectors of \mathbf{F} (having a desired feature) corresponding to the exact eigenvalue λ_k and let $\widehat{\mathbf{U}}_k$ be a matrix whose columns are the desired *exact* orthonormal eigenvectors of \mathbf{F} pertaining to λ_k .

3. A Direct Sequential Evaluation by Constrained Optimization Algorithm

For the k^{th} eigenspace of matrix \mathbf{F} , *exact* orthonormal eigenvectors $\widehat{\mathbf{u}}_s$, $s = 1, \dots, r_k$ will be sequentially evaluated such that they will be as close as possible - in the sense of Euclidian norm - to given *approximate* eigenvectors (having a desired feature) \mathbf{u}_s , $s = 1, \dots, r_k$. More specifically in the s^{th} stage $\widehat{\mathbf{u}}_s$ will be derived by minimizing

$$J_s = \|\mathbf{u}_s - \widehat{\mathbf{u}}_s\|_2^2 \tag{1}$$

subject to the constraints²

$$(\mathbf{F} - \lambda_k \mathbf{I})\hat{\mathbf{u}}_s = \mathbf{0}, \quad (2)$$

$$\hat{\mathbf{u}}_m^H \hat{\mathbf{u}}_s = 0 \quad , m = 1, \dots, s-1, \quad (3)$$

$$\|\hat{\mathbf{u}}_s\|^2 = 1. \quad (4)$$

Constraint (2) ensures that $\hat{\mathbf{u}}_s$ is an eigenvector of \mathbf{F} pertaining to λ_k . Constraint (3) satisfies the requirement that $\hat{\mathbf{u}}_s$ be orthogonal to the previously evaluated eigenvectors.

Constraint (4) is a normalization condition imposed such that $\hat{\mathbf{u}}_s$ has a unit Euclidian norm.

The set of linear constraints (2) and (3) can be compactly expressed as

$$\mathbf{C}_{s-1} \hat{\mathbf{u}}_s = \mathbf{0} \quad (5)$$

where

$$\mathbf{C}_{s-1} = \begin{bmatrix} \mathbf{F} - \lambda_k \mathbf{I} \\ \hat{\mathbf{u}}_1^H \\ \vdots \\ \hat{\mathbf{u}}_{s-1}^H \end{bmatrix}. \quad (6)$$

Since matrix \mathbf{C}_{s-1} is of dimension $(N + s - 1) \times N$, the homogeneous system of linear equations (5) has redundant constraints that can be eliminated by first applying the QR matrix decomposition technique resulting in

$$\mathbf{Q}_{s-1}^H \mathbf{C}_{s-1} \mathbf{E}_{s-1} = \begin{pmatrix} \mathbf{R}_{s-1} \\ \mathbf{0} \end{pmatrix}. \quad (7)$$

In the above equation \mathbf{Q}_{s-1} is a unitary matrix, \mathbf{E}_{s-1} is a permutation matrix³ and \mathbf{R}_{s-1} is a

$\rho_{s-1} \times N$ matrix where

$$\rho_{s-1} \equiv \text{rank}(\mathbf{C}_{s-1}). \quad (8)$$

² The superscripts ^T, ^{*}, ^H respectively denote the transpose, the complex conjugate and the Hermitian transpose (i.e. the complex conjugate transpose).

³ The symbol \mathbf{E}_{s-1} for the permutation matrix should not be confused with the symbol E_k for the eigenspace.

More specifically \mathbf{R}_{s-1} has the partitioned form

$$\mathbf{R}_{s-1} = (\mathbf{R}_a \quad \mathbf{R}_b) \quad (9)$$

where \mathbf{R}_a is a nonsingular upper triangular matrix of order ρ_{s-1} . Since the dimension of the eigenspace E_k (defined as the nullity of $(\mathbf{F} - \lambda_k \mathbf{I})$) is r_k , one concludes that

$$\text{rank}(\mathbf{F} - \lambda_k \mathbf{I}) = N - r_k. \quad (10)$$

Since the $(s-1)$ previously evaluated eigenvectors $\hat{\mathbf{u}}_m, m=1, \dots, s-1$ are orthonormal, the last $(s-1)$ rows of matrix \mathbf{C}_{s-1} are linearly independent. Consequently the rank of \mathbf{C}_{s-1} should satisfy

$$\rho_{s-1} \leq (N - r_k) + (s-1). \quad (11)$$

Heuristically the above inequality will hold as equality in almost all cases. The strict inequality will occur in the much unexpected case when one of the last $(s-1)$ rows of \mathbf{C}_{s-1} happens to be linearly dependent on the first N rows. Since $s \leq r_k$, one concludes that $\rho_{s-1} \leq (N-1)$. Substituting from (7) in (5) while exploiting the unitarity of \mathbf{Q}_{s-1} and \mathbf{E}_{s-1} , one gets

$$\mathbf{Q}_{s-1} \begin{pmatrix} \mathbf{R}_{s-1} \\ \mathbf{0} \end{pmatrix} \mathbf{E}_{s-1}^H \hat{\mathbf{u}}_s = \mathbf{0}. \quad (12)$$

Therefore the set of constraints (5) involving redundancy reduces to the set of linearly independent constraints

$$\mathbf{B}_{s-1} \hat{\mathbf{u}}_s = \mathbf{0} \quad (13)$$

where

$$\mathbf{B}_{s-1} = \mathbf{R}_{s-1} \mathbf{E}_{s-1}^H. \quad (14)$$

The constrained minimization problem defined by the objective (1) and the set of linearly independent linear constraints (13) and the single quadratic constraint (4) will be solved by the Lagrange multipliers technique. Augmenting the real criterion (1) by both the complex

vector constraint (13) and the real scalar constraint (4) using respectively a complex vector \mathbf{g} and a real scalar λ of Lagrange multipliers, one gets

$$J = \mathbf{u}_s^H \mathbf{u}_s + \hat{\mathbf{u}}_s^H \hat{\mathbf{u}}_s - \mathbf{u}_s^H \hat{\mathbf{u}}_s - \hat{\mathbf{u}}_s^H \mathbf{u}_s + \mathbf{g}^H \mathbf{B}_{s-1} \hat{\mathbf{u}}_s + \hat{\mathbf{u}}_s^H \mathbf{B}_{s-1}^H \mathbf{g} + \lambda (\hat{\mathbf{u}}_s^H \hat{\mathbf{u}}_s - 1). \quad (15)$$

The necessary condition for the minimization of J is

$$\nabla_{\hat{\mathbf{u}}_s} J = \mathbf{0} \quad (16)$$

where in evaluating the gradient vector w.r.t. $\hat{\mathbf{u}}_s^*$ one should view $\hat{\mathbf{u}}_s$ and $\hat{\mathbf{u}}_s^*$ as two different vectors, i.e. one should treat $\hat{\mathbf{u}}_s$ as a constant vector when operating with $\nabla_{\hat{\mathbf{u}}_s^*}$ [16]. From

(15), one gets

$$\nabla_{\hat{\mathbf{u}}_s} J = \hat{\mathbf{u}}_s - \mathbf{u}_s + \mathbf{B}_{s-1}^H \mathbf{g} + \lambda \hat{\mathbf{u}}_s. \quad (17)$$

Substituting the above equation in (16), one obtains

$$\hat{\mathbf{u}}_s = \frac{1}{(1+\lambda)} (\mathbf{u}_s - \mathbf{B}_{s-1}^H \mathbf{g}). \quad (18)$$

In order to evaluate the complex vector of Lagrange multipliers \mathbf{g} , one applies (13) to get

$$\frac{1}{(1+\lambda)} [\mathbf{B}_{s-1} \mathbf{u}_s - \mathbf{B}_{s-1} \mathbf{B}_{s-1}^H \mathbf{g}] = \mathbf{0}. \quad (19)$$

The linear independence of the rows of matrix \mathbf{B}_{s-1} implies the nonsingularity of $\mathbf{B}_{s-1} \mathbf{B}_{s-1}^H$.

Consequently the unique solution of (19) is

$$\mathbf{g} = (\mathbf{B}_{s-1} \mathbf{B}_{s-1}^H)^{-1} \mathbf{B}_{s-1} \mathbf{u}_s. \quad (20)$$

Substituting (20) in (18), one gets

$$\hat{\mathbf{u}}_s = \frac{1}{(1+\lambda)} \mathbf{A}_{s-1} \mathbf{u}_s \quad (21)$$

where

$$\mathbf{A}_{s-1} = \mathbf{I} - \mathbf{B}_{s-1} (\mathbf{B}_{s-1} \mathbf{B}_{s-1}^H)^{-1} \mathbf{B}_{s-1}^H. \quad (22-a)$$

Upon using (14), the above equation takes the form

$$\mathbf{A}_{s-1} = \mathbf{I} - \mathbf{E}_{s-1} \mathbf{R}_{s-1}^H (\mathbf{R}_{s-1} \mathbf{R}_{s-1}^H)^{-1} \mathbf{R}_{s-1} \mathbf{E}_{s-1}^H. \quad (22-b)$$

It can be proved that matrix \mathbf{A}_{s-1} is both Hermitian and idempotent, i.e.,

$$\mathbf{A}_{s-1}^H = \mathbf{A}_{s-1} \quad \text{and} \quad \mathbf{A}_{s-1}^2 = \mathbf{A}_{s-1}. \quad (23)$$

This implies that \mathbf{A}_{s-1} is a positive semidefinite matrix. In order to evaluate the real scalar Lagrange multiplier λ , one applies (4). Equations (4), (21) and (23) lead to

$$(1 + \lambda)^2 = \mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s. \quad (24)$$

From (21) and (24), one gets

$$\hat{\mathbf{u}}_s = \pm \frac{1}{\sqrt{\mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s}} \mathbf{A}_{s-1} \mathbf{u}_s. \quad (25)$$

Upon exploiting (23), the above result can be expressed as

$$\hat{\mathbf{u}}_s = \frac{1}{\|\mathbf{z}_s\|} \mathbf{z}_s \quad (26)$$

where

$$\mathbf{z}_s = \pm \mathbf{A}_{s-1} \mathbf{u}_s. \quad (27)$$

In order to select the right sign in (25) (or (27)) one substitutes (25) in (1) to get:

$$\begin{aligned} J_s &= \left\| \left(\mathbf{I} \mp \frac{\mathbf{A}_{s-1}}{\sqrt{\mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s}} \right) \mathbf{u}_s \right\|_2^2 \\ &= \mathbf{u}_s^H \left[\mathbf{I} \mp \frac{2}{\sqrt{\mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s}} \mathbf{A}_{s-1} + \frac{1}{\mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s} \mathbf{A}_{s-1} \right] \mathbf{u}_s \\ &= \|\mathbf{u}_s\|_2^2 \mp 2\sqrt{\mathbf{u}_s^H \mathbf{A}_{s-1} \mathbf{u}_s} + 1 \end{aligned} \quad (28)$$

The above form implies that J_s is minimized by selecting the negative sign in (28) which corresponds to the positive sign in (25). Therefore (27) should be replaced by:

$$\mathbf{z}_s = \mathbf{A}_{s-1} \mathbf{u}_s. \quad (29)$$

As an aside it will be shown in the Appendix that the above result can be reached by first setting aside the quadratic constraint (4), minimizing criterion (1) subject only to the linear constraints (13) and finally normalizing the solution vector - which will be proved to be (29) - in order to get (26).

Based on (26), (29), (22-b), (7) and (6), the Direct Sequential Evaluation by constrained Optimization Algorithm (DSEOA) for computing exact orthonormal eigenvectors of matrix \mathbf{F} - pertaining to the eigenvalue⁴ λ_k - that are the closest to given approximate eigenvectors (having a desired feature) can be summarized in the following steps:

1. Form matrix \mathbf{C} as

$$\mathbf{C} = \mathbf{F} - \lambda_k \mathbf{I}. \quad (30)$$

2. For $s = 1, \dots, r_k$:

- a) Perform the QR decomposition of \mathbf{C} with total pivoting:

$$\mathbf{Q}^H \mathbf{C} \mathbf{E} = \begin{pmatrix} \mathbf{R} \\ \mathbf{0} \end{pmatrix}. \quad (31)$$

Remark: Since matrix \mathbf{Q} will not be needed, the economy size version of the MATLAB command `qr` is used in performing this step.

- b) Compute \mathbf{z}_s as

$$\mathbf{z}_s = \left[\mathbf{I} - \mathbf{E} \mathbf{R}^H (\mathbf{R} \mathbf{R}^H)^{-1} \mathbf{R} \mathbf{E}^H \right] \mathbf{u}_s. \quad (32)$$

- c) Compute $\hat{\mathbf{u}}_s$ according to (26).

- d) Augment matrix \mathbf{C} by the row vector $\hat{\mathbf{u}}_s^H$.

4. Theoretical Equivalence of the DSEOA and GSA

⁴ The eigenvalue λ_k should not be confused with the Lagrange multiplier λ introduced in (15).

One objective of this section is to show that the DSEOA is theoretically equivalent to the Gram-Schmidt Algorithm (GSA) - contributed by Pei et al. [7] - despite being algorithmically quite distinct. This will be done by first showing that the DSEOA is theoretically equivalent to the Sequential Orthogonal Procrustes Algorithm (SOPA) contributed by Hanna et al. [10]. Another objective is to compare the DSEOA as presented in this paper with its counterpart contributed by Pei et al. [8].

Lemma:

The two algorithms DSEOA and GSA are theoretically equivalent.

Proof: In the SOPA, the target eigenvector $\hat{\mathbf{u}}_s$ is expressed as:

$$\hat{\mathbf{u}}_s = \mathbf{V}\mathbf{q}_s \quad , s = 1, \dots, r_k \quad (33)$$

where \mathbf{V} is an $N \times r_k$ matrix whose columns form orthonormal basis of E_k , i.e. those columns are *initial* orthonormal eigenvectors of matrix \mathbf{F} pertaining to λ_k . The vector \mathbf{q}_s is evaluated by minimizing criterion (1) subject to the constraints:

$$\mathbf{q}_m^H \mathbf{q}_s = 0 \quad , m = 1, \dots, s-1, \quad (34)$$

$$\|\mathbf{q}_s\|^2 = 1. \quad (35)$$

The first set of constraints of the DSEOA expressed by (2) ensures that $\hat{\mathbf{u}}_s$ is an eigenvector of \mathbf{F} corresponding to λ_k . In the SOPA the same constraint is satisfied by expressing $\hat{\mathbf{u}}_s$ as a linear combination of the vectors of an orthonormal basis of the eigenspace E_k as given by (33). The orthonormality of the columns of \mathbf{V} leads to:

$$\hat{\mathbf{u}}_m^H \hat{\mathbf{u}}_s = \mathbf{q}_m^H \mathbf{V}^H \mathbf{V} \mathbf{q}_s = \mathbf{q}_m^H \mathbf{q}_s. \quad (36)$$

Consequently the constraints (3) and (4) of the DSEOA are respectively equivalent to the constraints (34) and (35) of the SOPA. Therefore both the DSEOA and SOPA have

equivalent sets of constraints and since they have the same objective function (1), they are theoretically equivalent despite being algorithmically different.

Since it was proved in [10] that the SOPA and GSA are theoretically equivalent, the proof of the lemma is established.

(Q.E.D.)

It should be pointed out that the GSA and DSEOA are philosophically quite distinct despite being theoretically equivalent. In the GSA presented in [7], the *approximate* eigenvectors corresponding to one eigenspace (without being elements of it) are orthogonally projected on that space to get *exact* nonorthogonal eigenvectors which are next orthonormalized by applying the Gram-Schmidt procedure. In the DSEOA, the *exact* optimal orthonormal HGL eigenvectors pertaining to an eigenspace are directly and sequentially generated by solving a series of constrained minimization problems where in each problem the objective function is the squared Euclidean norm of the difference between a target exact eigenvector and an approximate one and where the constraints are the satisfaction of the definition of an exact eigenvector, orthogonality to previously generated ones and normalization of the target one.

Now one turns to the comparison between the method of last section and its counterpart contributed by Pei et al. in [8]. Although both methods sequentially evaluate the desired eigenvectors of \mathbf{F} using the same minimization criterion and the same set of constraints, it should be noticed that the present method is more computationally efficient and numerically accurate than the previous one for the following reasons:

- 1) In the DSEOA, orthonormal eigenvectors are computed for each eigenspace separately since the eigenspaces are mutually orthogonal by virtue of the unitarity of matrix \mathbf{F} . In the work of Pei et al. [8], all eigenvectors of \mathbf{F} are computed

sequentially which results in a larger number of redundant constraints at each stage since the orthonormality of the eigenspaces is not exploited.

- 2) In the work of Pei et al. [8], the set of constraints (2) was split into two sets of constraints by taking the real and imaginary parts and expressing them as separate constraints. This led to a larger number of redundant constraints at each stage of the sequential evaluation technique compared to the present DSEOA where the complex constraints are kept intact. It should be pointed out that although the vector constraints (2) and consequently (13) are complex, the cost function (15) has been formulated in such a way as to be real-valued.
- 3) In the present algorithm total pivoting is allowed in performing the QR matrix decomposition in (7), i.e. column interchange (as expressed by the permutation matrix \mathbf{E}_{s-1}) is allowed in order to enhance the accuracy and numerical stability of the computation. No such provision was incorporated in the work of Pei et al. [8].

5. Simulation Results

The general DSEOA of section 3 will be applied to the DFT matrix for which the number of eigenspaces is $K = 4$ and the columns of the matrices \mathbf{U}_k , $k = 1, \dots, 4$ defined in section 2 are samples of the Hermite-Gaussian functions [7]. Here the problem of the numerical determination of the rank ρ defined by (8) will first be discussed before proceeding to a comparative simulation study of various sequential techniques for generating HGL eigenvectors of the DFT matrix.

(A) Numerical Rank Determination

An examination of (7) – (9) shows that

$$\rho_{s-1} \equiv \text{rank}(C_{s-1}) = \text{rank}(R_{s-1}) = \text{rank}(R_a). \quad (37)$$

The challenging problem is that of the numerical evaluation of ρ_{s-1} . In order to facilitate the discussion three different symbols will be used. First the rank determined by the built-in MATLAB function $\text{rank}(C)$ will be denoted by ρ_{matlab} . Second the rank determined based on the results obtained by applying the QR matrix decomposition technique will be denoted by ρ_{QR} . Finally based on the discussion preceding and following (11), the heuristic value of the rank will be denoted by $\rho_{heuristic}$ and is given by:

$$\rho_{heuristic} = (N - r_k) + (s - 1). \quad (38)$$

MATLAB uses a method based on the singular value decomposition and the rank ρ_{matlab} is evaluated as the number of singular values exceeding the tolerance given by:

$$\text{tolerance} = \max(\text{size}(C)) * \text{largest singular value} * \text{eps} \quad (39)$$

where $\max(\text{size}(C)) = N + s - 1$ (as can be seen from (6)) and eps is the built-in MATLAB constant called the floating-point relative accuracy and defined as the distance from 1.0 to the next larger double-precision number⁵, i.e. $\text{eps} = 2^{(-52)} \cong 2.22e - 016$. Although the MATLAB function rank uses the most reliable method for rank determination, it is also the most time consuming.

Needlessly to say, having the QR decomposition of matrix C_{s-1} in (7) one can immediately determine the rank as the number of rows of matrix R_{s-1} . The main numerical problem is that after performing the QR decomposition, one only gets the R.H.S. of (7) and one has to identify matrix R_{s-1} and the zero matrix (whose elements are practically negligibly nonzero due to the effect of the accumulated round-off error). In case of performing the QR decomposition with the Total Pivoting (TP) option the absolute values of the diagonal

⁵ Here the MATLAB notation is used where $e - 016$ stands for $10^{(-16)}$.

elements of the resulting R.H.S. matrix in (7) will appear in descending absolute values. Consequently the number of those diagonal elements whose absolute values pass a certain threshold will give the numerical rank ρ_{QR} . The threshold will be taken as

$$threshold = (N + s - 1) * DRR(1) * mtol * eps \quad (40a)$$

where $DRR(1)$ is the absolute value of the first diagonal element of the R.H.S. of (7). This choice of the threshold is based on the same sound reasoning adopted in (39). Moreover the arbitrary multiplying factor $mtol$ appearing in (40a) has been introduced in order to allow the user more flexibility in coping with the challenging numerical rank determination problem. As a rule of thumb it has been found after tedious experimentation that the value $mtol = 1e006$ suffices in most cases.

In case of performing the QR decomposition with the Non Total Pivoting (NTP) option, matrix \mathbf{E}_{s-1} in (7) will be replaced by the identity matrix and the diagonal elements of the resulting R.H.S. matrix will not appear in descending absolute values. Consequently the appropriate threshold to be adopted in this case is:

$$threshold = (N + s - 1) * \max(DRR) * mtol * eps \quad (40b)$$

where $\max(DRR)$ is the maximum of the absolute values of the diagonal elements of the R.H.S. matrix in (7).

Now one turns to the actual simulation results obtained using ρ_{matlab} and ρ_{QR} :

- (i) One applies the DSEOA with both the total pivoting (TP) and non total pivoting (NTP) options taking ρ_{matlab} as the adopted rank. Expectedly the computation time⁶ in the TP case is longer than its counterpart in the NTP case as can be observed in Table 1. Surprisingly it has been found that in both cases $\rho_{heuristic} = \rho_{matlab}$ for values of the order N of the DFT matrix \mathbf{F} as large as 512.

⁶ The computation was performed on a PC with Intel processor Core 2 Duo having speed 2.41 GHz with 1.00 GB of RAM.

The conclusion is that one can take $\rho_{heuristic}$ as the reliable value of the rank for values of N as large as 512.

- (ii) One repeats (i) employing only ρ_{QR} . Guided by the above finding regarding the reliability of $\rho_{heuristic}$, one experiments with the selection of the multiplying factor $mtol$ appearing in (40a) and (40b) and affecting the value of the threshold and consequently the value of ρ_{QR} . For each value of the order N of matrix \mathbf{F} one counts the sum of the number of stages n of the sequential technique DSEOA in all eigenspaces where $\rho_{QR} \neq \rho_{heuristic}$. More specifically, let n_g be the number of cases where $\rho_{QR} > \rho_{heuristic}$ and n_s be the number of cases where $\rho_{QR} < \rho_{heuristic}$ and let $n = n_g + n_s$. Table 2 provides all the results for values of N up to 512 and values of $mtol$ ranging from 1 to $1e013$. The most striking observation is the definite merit of the TP option over the NTP option. Adopting the TP option and concentrating on the choice of the value of $mtol$, one should avoid values as small as 1 and as large as $1e013$. It seems that $mtol = 1e006$ is a reasonable choice. It should be emphasized that having $n_g \neq 0$ is not acceptable at all because it means that the adopted value of the rank ρ_{QR} is larger than the reliable value and consequently in identifying matrix R_{s-1} in (7) some almost zero rows will be included at the bottom resulting in having an almost singular matrix RR^H to be inverted in (32).
- (iii) Based on the experience gained above, the DSEOA with the total pivoting option is applied and ρ_{QR} is evaluated using $mtol = 1e006$. The computation time of the algorithm is given in Table 3. Quite interestingly it has been found that $\rho_{heuristic} = \rho_{QR}$ for values of N as large as $N = 2048$.

(B) A Comparative Simulation Study

Hermite-Gaussian-like eigenvectors of the DFT matrix are generated using the following five sequential techniques:

- 1) The DSEOA delineated in section 3 and applied with the total pivoting option while taking ρ_{QR} as the adopted rank identified using the multiplying factor $mtol = 1e006$.
- 2) The *Gram-Schmidt algorithm* proposed by Pei et al. [7] where the initial basis of the eigenspaces are obtained by the eigendecomposition of the nearly tridiagonal matrix \mathbf{S} in the manner elaborated upon by Candan et al. [4]. (This technique will be referred to as GSA1).
- 3) The *Gram-Schmidt algorithm* of Pei et al. [7] implemented by the direct utilization of the orthogonal projection matrices of matrix \mathbf{F} on its eigenspaces as proposed by Hanna et al. [11]. (This technique will be referred to as GSA2).
- 4) The *sequential orthogonal procrustes algorithm* proposed by Hanna et al. [10] where the initial basis are generated as in (2) above. (This technique will be referred to as SOPA1).
- 5) The *sequential orthogonal procrustes algorithm* implemented by the direct utilization of the projection matrices without having to first generate initial basis [11]. (This technique will be referred to as SOPA2).

The computation time in seconds of the eigenvectors using the five sequential techniques is given in Table 4 for various values of the order⁷ N .

Since the three methods - DSEOA, GSA and SOPA - were shown in section 4 to be theoretically equivalent, the five sequential techniques mentioned above are supposed to give identical results in the absence of the round off error which is unavoidable. The norm of the

⁷ The computation is performed on a PC where some system related tasks are unavoidably concurrently taking place. This interprets the unexpected decrease in the computation time of the GSA1 for $N = 64$ and 128 compared to its value for $N = 32$. It should be mentioned that the discrepancy between the computation time of the DSEOA given in the second column of Table 4 and that given in Table 3 is attributed to the same reason.

approximation error vectors $\mathbf{e}_m \equiv (\hat{\mathbf{u}}_m - \mathbf{u}_m)$, $m = 1, \dots, N$ between the exact and approximate eigenvectors – which is the square root of the minimization criterion J_m defined by (1) – is plotted for the five sequential techniques. It has been found that there is no noticeable difference among them for values of the order N up to 128. For larger values of N , one begins to notice some differences which grow with N . Fig. 1 shows the plots of the DSEOA and GSA1 and Fig. 2 shows the plots of the DSEOA and SOPA1 for $N = 512$. The discrepancy between the two plots in each figure is pronounced only for values of the index m near N .

One will next explore the issue of deciding which technique is more numerically stable. Let matrix $\hat{\mathbf{U}}$ be the unitary modal matrix of \mathbf{F} . The columns of $\hat{\mathbf{U}}$ are obtained from the columns of the four matrices $\hat{\mathbf{U}}_k$, $k = 1, \dots, 4$ mentioned near the end of section 2. The orthonormality error matrix is defined by:

$$\mathbf{C} = \hat{\mathbf{U}}^H \hat{\mathbf{U}} - \mathbf{I}. \quad (41)$$

In the absence of the computation round off error – which will never be the case – the above matrix should be identically zero. In order to compare the numerical accuracy of the five sequential techniques under investigation in this comparative study, two measures of the above matrix – namely the maximum element in absolute value and the Frobenius norm – are computed and given respectively in Tables 5 and 6. A rapid examination of those two tables reveals that the orthonormality error is negligible for the first five techniques for values of N up to 128. The main conclusion is that the DSEOA is the most numerically robust technique among the five sequential techniques since its orthonormality error is negligible for values of N as large as 1024. This is the distinct advantage that one gains in the DSEOA case in return to the long computation time noticeable in Table 4. A second conclusion is that for the GSA1, GSA2, SOPA1 and SOPA2 the orthonormality error is felt starting at $N = 256$.

Only for the sake of extending the comparison, the *orthogonal procrustes algorithm* (OPA) is included in this comparative simulation study although it is based on a completely

different rationale since it is a *batch* – rather than a *sequential* – technique. More specifically the simulation study also covers the following two *batch* techniques:

- 1) The *orthogonal procrustes algorithm* [7] where the initial basis of the eigenspaces are obtained by the eigendecomposition of the nearly tridiagonal matrix \mathbf{S} in the manner elaborated upon in [4]. (This technique will be referred to as OPA1).
- 2) The *orthogonal procrustes algorithm* [7] implemented by the direct utilization of the orthogonal projection matrices of matrix \mathbf{F} on its eigenspaces as proposed in [11]. (This technique will be referred to as OPA2).

The results pertaining to OPA1 and OPA2 are included as the last two columns of Tables 4-6 and the plot pertaining to OPA1 is superimposed on Figs 1-2. By examining the approximation error depicted in those two figures one finds that the *sequential* methods have the advantage that the threshold value of the index m where the error starts to be noticeable is larger than its counterpart for the OPA. On the other hand the OPA has the merit that its maximum approximation error is smaller than its counterpart in the sequential methods.

6. Conclusion

A technique is proposed for the direct sequential evaluation of optimal HGL orthonormal eigenvectors of the DFT matrix \mathbf{F} by constrained optimization. The orthonormality of the eigenspaces pertaining to distinct eigenvalues is exploited in decoupling the problem such that the orthonormal eigenvectors of each eigenspace are separately evaluated thus reducing the number of constraints. Total pivoting is employed in performing the QR matrix decomposition – needed for singling out the linearly independent constraints – with the objective of enhancing the numerical stability of the computation. The contributed DSEOA has been proved to be theoretically equivalent to both the GSA and SOPA although the three

techniques are algorithmically quite distinct. The extensive comparative simulation study has shown that the DSEOA is the most numerically robust method among all sequential techniques thus justifying its relatively long computation time.

Appendix A: (Minimizing (1) subject to (13) setting aside (4))

Since the quadratic constraint (4) will be set aside for a while, the solution of the constrained minimization problem defined by the objective (1) and the independent constraints (13) will be denoted by \mathbf{x}_s rather than $\hat{\mathbf{u}}_s$.

Statement of the problem: Determine the vector \mathbf{x}_s which minimizes the criterion:

$$J_s = \|\mathbf{u}_s - \mathbf{x}_s\|_2^2 \quad (\text{A-1})$$

subject to the set of linearly independent constraints:

$$\mathbf{B}_{s-1}\mathbf{x}_s = \mathbf{0}. \quad (\text{A-2})$$

Solution: Augmenting criterion (A-1) by the constraints (A-2) using a vector \mathbf{g} of Lagrange multipliers, one gets

$$J_c = \mathbf{u}_s^H \mathbf{u}_s + \mathbf{x}_s^H \mathbf{x}_s - \mathbf{u}_s^H \mathbf{x}_s - \mathbf{x}_s^H \mathbf{u}_s + \mathbf{g}^H \mathbf{B}_{s-1} \mathbf{x}_s + \mathbf{x}_s^H \mathbf{B}_{s-1}^H \mathbf{g}. \quad (\text{A-3})$$

The necessary conditions for the minimization of J_c are

$$\nabla_{\mathbf{x}_s^*} J_c = \mathbf{0} \quad (\text{A-4})$$

where in evaluating the gradient vector w.r.t. \mathbf{x}_s^* one should view \mathbf{x}_s and \mathbf{x}_s^* as two different vectors, i.e. one should treat \mathbf{x}_s as a constant vector when operating with $\nabla_{\mathbf{x}_s^*}$ [16]. From (A-3), one gets

$$\nabla_{\mathbf{x}_s^*} J_c = \mathbf{x}_s - \mathbf{u}_s + \mathbf{B}_{s-1}^H \mathbf{g}. \quad (\text{A-5})$$

Substituting from the above equation in (A-4), one obtains

$$\mathbf{x}_s = \mathbf{u}_s - \mathbf{B}_{s-1}^H \mathbf{g}. \quad (\text{A-6})$$

In order to evaluate the Lagrange multipliers vector \mathbf{g} , one applies (A-2) to get

$$\mathbf{B}_{s-1} \mathbf{u}_s - \mathbf{B}_{s-1} \mathbf{B}_{s-1}^H \mathbf{g} = \mathbf{0}. \quad (\text{A-7})$$

The linear independence of the rows of matrix \mathbf{B}_{s-1} implies the nonsingularity of $\mathbf{B}_{s-1}\mathbf{B}_{s-1}^H$.

Consequently the unique solution of (A-7) is

$$\mathbf{g} = \left(\mathbf{B}_{s-1}\mathbf{B}_{s-1}^H\right)^{-1}\mathbf{B}_{s-1}\mathbf{u}_s. \quad (\text{A-8})$$

Substituting (A-8) in (A-6), one gets

$$\mathbf{x}_s = \left[\mathbf{I} - \mathbf{B}_{s-1}^H\left(\mathbf{B}_{s-1}\mathbf{B}_{s-1}^H\right)^{-1}\mathbf{B}_{s-1}\right]\mathbf{u}_s. \quad (\text{A-9})$$

Upon comparing the above equation with (29) and (22-a), one concludes that

$$\mathbf{x}_s = \mathbf{z}_s. \quad (\text{A-10})$$

Therefore upon applying the normalization condition (26) - which is equivalent to constraint (4) - one gets the same solution obtained in section 3.

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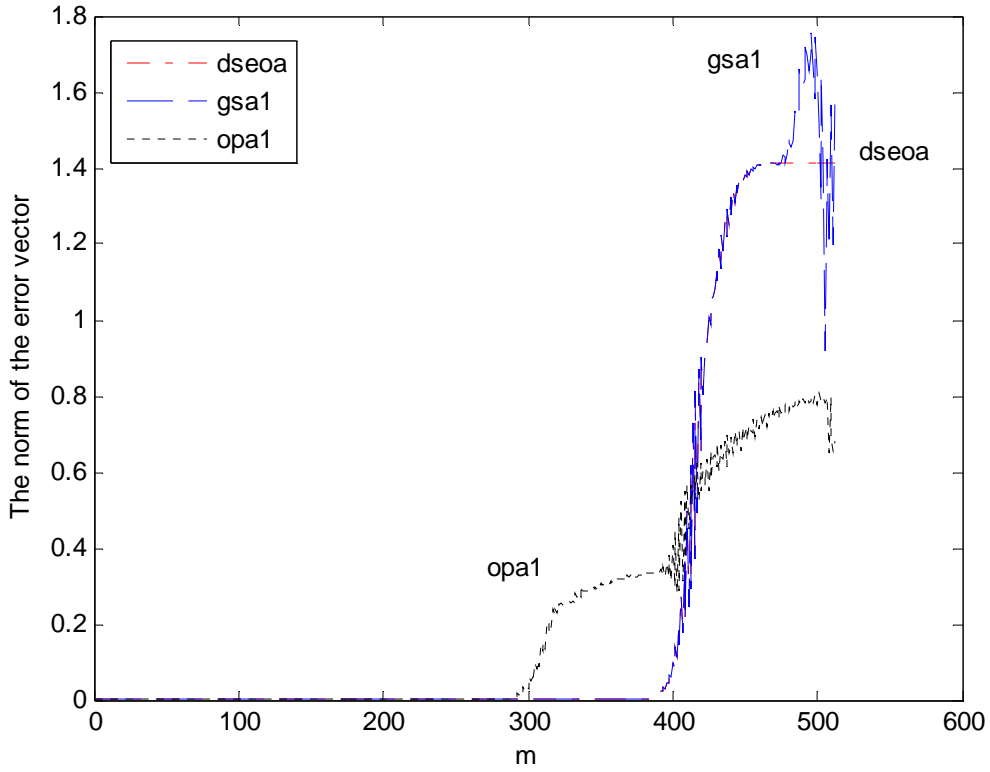


Fig. 1: The norm of the error vectors $\mathbf{e}_m \equiv (\hat{\mathbf{u}}_m - \mathbf{u}_m)$, $m = 1, \dots, N$ between the exact and approximate eigenvectors using the DSEO, GSA1 and OPA1 for $N = 512$.

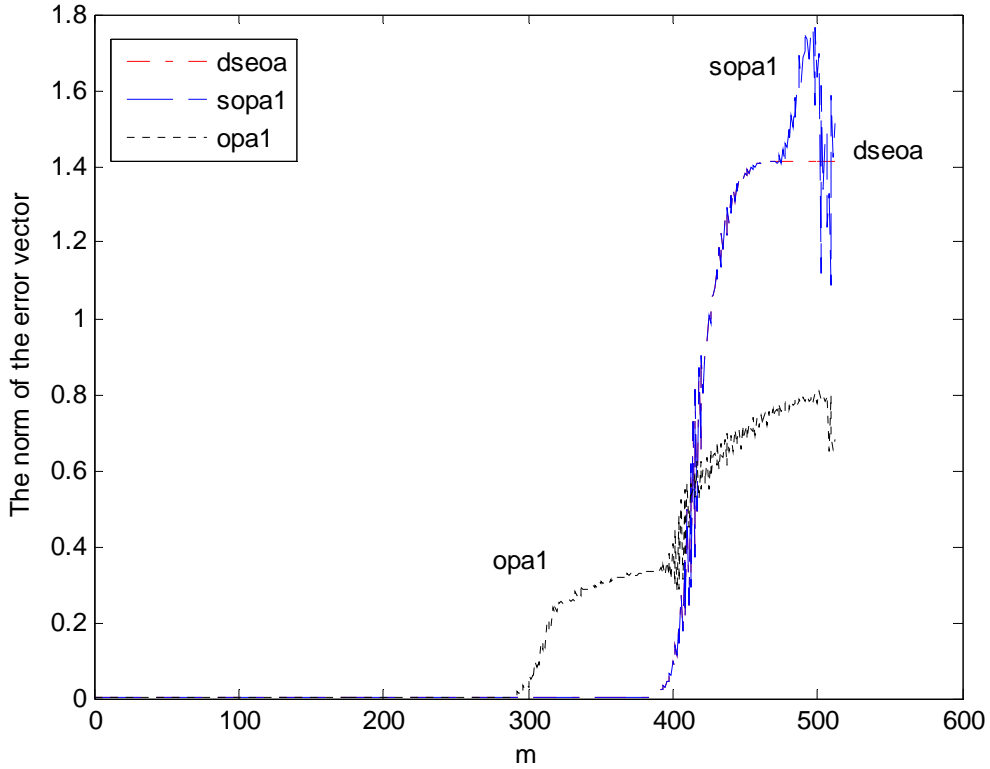


Fig. 2: The norm of the error vectors $\mathbf{e}_m \equiv (\hat{\mathbf{u}}_m - \mathbf{u}_m)$, $m = 1, \dots, N$ between the exact and approximate eigenvectors using the DSEO, SOPA1 and OPA1 for $N = 512$.

Table 1: The computation time (in seconds) of the DSEOA with both the total pivoting (TP) and non total pivoting (NTP) options where ρ_{matlab} is adopted.

N	DSEOA-TP	DSEOA-NTP
32	0.15625	0.09375
64	0.6875	0.578125
128	7.9375	7.609375
256	118.07813	116.82813
512	1958.8594	1848.6875

Table 2: The number of stages n of the DSEOA where $\rho_{QR} \neq \rho_{heuristic}$ for both the total pivoting (TP) and non total pivoting (NTP) options versus the order N of matrix \mathbf{F} and the multiplying factor $mtol$. (A blank cell means a zero value).

$mtol$	N	The case of total pivoting (TP)			The case of non total pivoting (NTP)		
		n	n_g	n_s	n	n_g	n_s
1	32	2	2		32	32	
	64	25	25		64	64	
	128	102	102		128	128	
	256	223	223		256	256	
	512	510	510		512	512	
1e002	32				5	5	
	64				26	26	
	128				113	113	
	256				256	256	
	512				512	512	
1e004	32				2	2	
	64				25	25	
	128				119	119	
	256				255	255	
	512				512	512	
1e006	32						
	64				30	30	
	128				115	114	1
	256				250	220	30
	512				508	418	90

1e008	32						
	64				36	12	24
	128				118	74	44
	256				255	157	98
	512				511	300	211
1e010	32						
	64				35		35
	128				116	41	75
	256				251	84	167
	512				508	124	384
1e012	32				15		15
	64				50		50
	128				117		117
	256				248	25	223
	512				512	1	511
1e013	32				23		23
	64				58		58
	128				124		124
	256	256		256	256		256
	512	512		512	512		512

Table 3: The computation time (in seconds) of the DSEOA with the total pivoting (TP) option where ρ_{QR} is adopted.

N	DSEOA-TP
32	0.125
64	0.515625
128	5.765625
256	81.546875
512	1296.6563
1024	20010.953
2048	322546.94

Table 4: The computation time (in seconds) of the eigenvectors.

N	DSEOA	GSA1	GSA2	SOPA1	SOPA2	OPA1	OPA2
32	0.062500	0.062500	0.000000	0.015625	0.015625	0.000000	0.015625
64	0.406250	0.015625	0.000000	0.015625	0.015625	0.015625	0.015625
128	5.656250	0.031250	0.015625	0.062500	0.062500	0.046875	0.015625
256	81.968750	0.234375	0.093750	0.500000	0.796875	0.203125	0.109375
512	1297.078100	2.734375	0.687500	6.781250	9.125000	2.546875	0.812500
1024	20227.859000	24.750000	6.406250	90.703125	129.640630	21.781250	6.046875

Table 5: The maximum orthonormality error.

N	DSEOA	GSA1	GSA2	SOPA1	SOPA2	OPA1	OPA2
32	1.75601E-15	8.07E-16	1.52E-15	2E-15	1.8E-15	2.77556E-15	2.22E-15
64	2.87701E-15	3.69E-15	1.68E-14	4.1E-15	2.01E-14	3.9968E-15	9.77E-15
128	3.04292E-14	2.96E-12	6.15E-12	3.3E-12	1.39E-11	3.9968E-15	8.08E-13
256	1.00472E-11	0.907323	0.948369	0.487144	0.764895	3.33067E-15	1.03E-08
512	6.2374E-07	0.999726	0.99967	0.999694	0.999433	6.66134E-15	0.066633
1024	1.71655E-06	0.996934	0.997635	0.996096	0.996	6.21725E-15	0.095487

Table 6: The Frobenius norm of the orthonormality error matrix.

N	DSEOA	GSA1	GSA2	SOPA1	SOPA2	OPA1	OPA2
32	1.60369E-14	3.92E-15	1.18E-14	5.88E-15	1.33E-14	8.25223E-15	1.35E-14
64	4.65985E-14	1.48E-14	8.77E-14	1.66E-14	1.11E-13	1.63735E-14	8.73E-14
128	2.57574E-13	4.89E-12	1.67E-11	5.12E-12	2.77E-11	2.8328E-14	1.21E-11
256	7.32889E-11	1.289249	1.44861	0.780886	1.180467	5.19285E-14	1.63E-07
512	4.90945E-06	18.81388	18.64308	19.15301	19.11718	9.74772E-14	2.840916
1024	2.81776E-05	50.98267	50.21463	48.26681	48.15584	1.98156E-13	6.325207



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