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Chapter 3

ON THE BEST LEAST SQUARES FIT TO A MATRIX AND ITS APPLICATIONS

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Abstract

The best least squares fit $\mathcal{L}_A$ to a matrix A in a space $\mathcal{L}$ can be useful to improve the rate of convergence of the conjugate gradient method in solving systems $A\mathbf{x} = \mathbf{b}$ as well as to define low complexity quasi-Newton algorithms in unconstrained minimization. This is shown in the present paper with new important applications and ideas. Moreover, some theoretical results on the representation and on the computation of $\mathcal{L}_A$ are investigated.

1 Introduction

In this paper the concept of matrix approximation is linked to a general strategy or to an idea which has been proposed in a number of previous papers and tested for several problems of numerical linear algebra and numerical optimization. The idea is simply the following one: reduce a computational problem involving linear operators non sufficiently structured to a framework where only matrices with a special structure are present, and where the essential computation consists, finally, in a small number of fast transforms. This reduction has been used in different contexts, and is turned out to be an effective tool for analyzing the complexity and improving the efficiency of algorithms. For instance, the very special properties of matrix algebras of Jacobi type are used in [7] to calculate the eigenvalues of symmetric Toeplitz matrices and in [8], [47] to find the multiplicative complexity of a set of Toeplitz bilinear forms. Circulant, Jacobi, and Hartley-type matrices are usually exploited in preconditioning techniques [42], [18], [9], [16], [21], [30]. In displacement theory [39],

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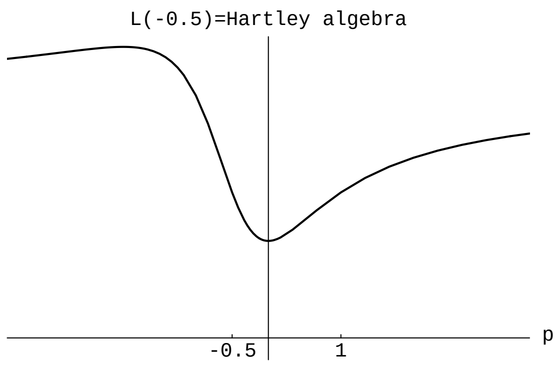

Figure 1: The graphic of $\|\mathcal{L}(p)_T - T\|_F^2$: Hartley is not optimal

[38], one can solve a linear system $A\mathbf{x} = \mathbf{b}$ by representing A^{-1} as the sum of a small number of products of matrices belonging to Hessenberg [29], [12], or more general [23], [4], algebras. Finally, in quasi-Newton algorithms for unconstrained minimization, a crucial reduction of (time and space) complexity is obtained by iterations involving special Hessian approximations diagonalized by fast transforms [25], [11].

The reduction of non sufficiently structured problems to structured ones is performed via matrix approximation in Frobenius norm, i.e. by replacing a matrix A by its best least squares (l.s.) fit $\mathcal{L}_A$, where the matrix $\mathcal{L}_A$ belongs to a fixed algebra $\mathcal{L}$. Part of the paper is devoted to a review and to a further investigation of previous results obtained in [30], [25]. Moreover, several new results, applications and ideas are presented.

The seed of the research which finally resulted in [30] and then in [25], consisted in the graphic of Figure 1. It represents the error in approximating a 3×3 symmetric Toeplitz matrix $T = (t_{i-j})$ in a class $\mathcal{L}(p)$, $p \in \mathbb{R}$, of matrix algebras studied in [23], or, more precisely, the rational function in the equality

$$\min_{X \in \mathcal{L}(p)} \|X - T\|_F^2 \equiv \|\mathcal{L}(p)_T - T\|_F^2 = \frac{10p^2 + 4p + 4}{9(p^2 + p + 1)}(t_1 - t_2)^2, \quad p \in \mathbb{R}, \tag{1.1}$$

where $\|X\|_F = \sqrt{\mathrm{tr}(X^*X)}$ is the Frobenius norm of X.

The Hartley algebra $\mathcal{H}$, previously introduced in [9], is a member of $\mathcal{L}(p)$, and corresponds to the value $p = -1/2$. In [9] it is shown that $\mathcal{H}_T$, i.e. the best least squares (l.s.) fit to T in $\mathcal{H}$, can be an efficient preconditioner in solving Toeplitz systems $T\mathbf{x} = \mathbf{b}$ by the conjugate gradient (CG) metod. Figure 1 shows clearly that T can be approximated better by picking up in the class $\mathcal{L}(p)$ an algebra different from $\mathcal{H} = \mathcal{L}(-\frac{1}{2})$ and precisely the new matrix algebra $\eta = \mathcal{L}(0)$. This obviously suggested the study of η_T and other matrices $\mathcal{L}(p)_T$ as new preconditioners.

The contents of this paper are described here below.

In Section 2, we point out the main properties of the best least squares fit $\mathcal{L}_A$ to a $n \times n$ matrix A. Some of the remarks included are new and all of them are useful in computing $\mathcal{L}_A$. Several examples and problems are reported. Two possible applications of $\mathcal{L}_A$ are considered in the next sections.

In Section 3, $\mathcal{L}_A$ is exploited as a preconditioner in solving positive definite linear systems $A\mathbf{x} = \mathbf{b}$ by the CG method. The space $\mathcal{L}$ is a diagonal space $sd\,U = \{Ud(\mathbf{z})U^* : \mathbf{z} \in \mathbb{C}^n\}$, i.e.

$$P^{-1}A\mathbf{x} = P^{-1}\mathbf{b}, \quad P = \mathcal{L}_A = Ud(\mathbf{z}_A)U^*$$

where U is a unitary matrix and $d(\mathbf{z}) = \mathrm{diag}(z_i, i = 1, \ldots, n)$. In particular, $\mathcal{L}$ can be the algebra $\mathcal{H}$, the algebra η or, more in general, a *Hartley-type* matrix algebra. Recall that the set of Hartley-type algebras was proposed in [10] as the Hartley counterpart of the known classification of Jacobi transforms/algebras. Theoretical and numerical results on the use of $\mathcal{L}_A$ as a preconditioner are reported in the cases $A = T$, T=symmetric Toeplitz [30] and $A = T^T T$, T=generic (non symmetric) Toeplitz.

In Section 4, $\mathcal{L}_A$ is involved in a novel low complexity quasi-Newton procedure for the unconstrained minimization of a function $f : \mathbb{R}^n \to \mathbb{R}$. The new algorithm is based on the following approximation of the Hessian $\nabla^2 f(\mathbf{x}_{k+1})$ in terms of the updating function (4.1):

$$B_{k+1} = \varphi(U_k d(\mathbf{v})U_k^*, \mathbf{s}_k, \mathbf{y}_k), \quad \mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k,\ \mathbf{y}_k = \nabla f(\mathbf{x}_{k+1}) - \nabla f(x_k)$$

where the unitary matrix U_k and the vector $\mathbf{v}$ are defined in terms of $\mathbf{s}_{k-1}$, $\mathbf{y}_{k-1}$ and a suitable vector $\mathbf{w}$ as follows:

1. $\mathbf{w}$ is such that $U_{k-1}d(\mathbf{w})U_{k-1}^* = \mathcal{L}_{B_k}^{k-1}$ with $\mathcal{L}^{k-1} = sd\,U_{k-1}$,
2. U_k is such that $U_k d(\mathbf{z})U_k^* \mathbf{s}_{k-1} = \mathbf{y}_{k-1}$ for some vector $\mathbf{z}$ close to $\mathbf{w}$, and
3. $\mathbf{v} = \mathbf{w}$ or $\mathbf{v} = \mathbf{z}$.

Item (1) implies that the eigenvalues of the matrix $A_k := U_k d(\mathbf{w})U_k^*$ are strictly related to the eigenvalues of B_k and can be easily calculated. By item (2) the structure of $\mathcal{L}^k = \{U_k d(\mathbf{z})U_k^* : \mathbf{z} \in \mathbb{C}^n\}$ is such that $A_k' := U_k d(\mathbf{z})U_k^*$ shares with B_k the property of mapping $\mathbf{s}_{k-1}$ into $\mathbf{y}_{k-1}$. Thus, the updated matrix, $U_k d(\mathbf{v})U_k^*$, inherites from B_k both spectral and structural properties. Moreover, since iterations involve only $\mathbf{v}$ and since U_k is the product of two Householder matrices, all computations can be written in terms of single indexed arrays only. Thus, $O(n)$ arithmetic operations per step and $O(n)$ memory allocations are sufficient to implement the algorithm. So, the most significant properties of the $\mathcal{L}QN$ methods [25], [11], [24], and of the more recent $\mathcal{L}^k QN$ methods [27] are inherited by the new algorithm.

2 The Best Least Squares Fit to a Matrix

Let $J_1,\ J_2, \ldots, J_m$ be m linearly independent $n \times n$ matrices and consider the $m \times m$ hermitian matrix B with entries

$$b_{ij} = (J_i, J_j) = \sum_{r,s=1}^{n} \overline{[J_i]}_{rs}[J_j]_{rs}. \tag{2.1}$$

From the identity

$$\mathbf{x}^* B\mathbf{x} = \sum_{r,s=1}^{n} \left| \sum_{j=1}^{m} x_j [J_j]_{rs} \right|^2, \quad \mathbf{x} \in \mathbb{C}^m, \tag{2.2}$$

one deduces that B is a hermitian positive definite matrix.

Problem 1: Given a $m \times m$ hermitian positive definite matrix B, is it possible to define m linearly independent $n \times n$ matrices $J_1,\ J_2,\ \ldots,\ J_m$ such that $(J_i, J_j) = [B]_{ij}$?

The matrix B in (2.1) arises when calculating the *best least squares (l.s) fit* to a matrix A in the space $\mathcal{L}$ spanned by the J_k, i.e. when solving the following

Problem 2.1 *Find the complex numbers α_k for which*

$$\| \sum_{k=1}^{m} \alpha_k J_k - A\|_F \leq \| \sum_{k=1}^{m} \beta_k J_k - A\|_F, \quad \forall \beta_k \in \mathbb{C}, \tag{2.3}$$

where A is any fixed $n \times n$ matrix and $\|\cdot\|_F$ is the Frobenius norm.

In fact, by the Hilbert projection theorem, Problem 2.1 is well posed, i.e. there is a unique vector $\alpha = [\alpha_1\ \alpha_2 \cdots\ \alpha_m]$ satisfying the inequality (2.3) or, equivalently, the orthogonality conditions

$$(J_i, \sum_{k=1}^{m} \alpha_k J_k - A) = 0, \quad i = 1, \ldots, m. \tag{2.4}$$

Such vector α is

$$\alpha = B^{-1}\mathbf{c}, \quad c_i = (J_i, A) = \sum_{r,s=1}^{n} \overline{[J_i]}_{rs}[A]_{rs}. \tag{2.5}$$

Moreover, since $\| \sum_{k=1}^{n} \beta_k J_k - A\|_F^2 = \beta^* B \beta - 2\,\mathrm{Re}(\beta^* \mathbf{c}) + \|A\|_F^2$, one has the following expressions for the error

$$\| \sum_{k=1}^{n} \alpha_k J_k - A\|_F^2 = \|A\|_F^2 - \alpha^* B \alpha = \|A\|_F^2 - \| \sum_{k=1}^{n} \alpha_k J_k\|_F^2. \tag{2.6}$$

Finally, observe that if A is real (hermitian), then also $\sum_{k=1}^{n} \alpha_k J_k$ is real (hermitian), provided that $J_k = \overline{J_k}$ ($J_k^* \in$ Span$\{J_1, \ldots, J_n\}$).

Thus the computations required in order to solve Problem 2.1 are:

1. Calculate the inner products $c_i = (J_i, A)$
2. Calculate B and solve the system $B\mathbf{z} = \mathbf{c}$

The error may be calculated via (2.6).

Definition 2.2 *Call $\mathcal{L}_A$ the matrix $\sum_{k=1}^{m} \alpha_k J_k$ satisfying* (2.3), (2.4). *We have obviously*

$$\mathcal{L}_A = \sum_{k=1}^{m} [B^{-1}\mathbf{c}]_k J_k. \tag{2.7}$$

Example 1. An n-dimensional space $\mathcal{L}$ often used in numerical linear algebra is the space $\tau = \text{Span}\{J_1, \dots, J_n\}$ where

$$J_k = \begin{bmatrix} 0 & \cdots & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & & \iddots & 1 & 0 & 1 & \ddots & & & \vdots \\ \vdots & \iddots & \iddots & \iddots & 1 & \ddots & \ddots & \ddots & & \vdots \\ 0 & 1 & \iddots & \iddots & & \ddots & \ddots & \ddots & \ddots & \vdots \\ 1 & 0 & 1 & & & & \ddots & \ddots & 1 & 0 \\ 0 & 1 & \ddots & \ddots & & & & 1 & 0 & 1 \\ \vdots & \ddots & \ddots & \ddots & \ddots & & \iddots & \iddots & 1 & 0 \\ \vdots & & \ddots & \ddots & \ddots & 1 & \iddots & \iddots & \iddots & \vdots \\ \vdots & & & \ddots & 1 & 0 & 1 & \iddots & & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & 1 & 0 & \cdots & \cdots & 0 \end{bmatrix}$$

with $\mathbf{e}_1^T J_k = \mathbf{e}_k^T$. For the definition and the first applications of τ see [3], [47], [48], [7], [8]. Notice that $J_k = J_{k-1}J_2 - J_{k-2}$, J_1 is the identity matrix I and J_n is the reversing matrix J. For $n = 4$ one calculates

$$B = \begin{bmatrix} 4 & 0 & 2 & 0 \\ 0 & 6 & 0 & 2 \\ 2 & 0 & 6 & 0 \\ 0 & 2 & 0 & 4 \end{bmatrix}, \quad B^{-1} = \frac{1}{10} \begin{bmatrix} 3 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 \\ -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 3 \end{bmatrix}. \tag{2.8}$$

It follows that the best approximation of A in $\tau = \text{Span}\{J_1, J_2, J_3, J_4\}$ is

$$\begin{aligned} \textstyle\sum_{k=1}^4 \alpha_k J_k \quad &= \quad \tfrac{1}{10}[(3c_1 - c_3)J_1 + (2c_2 - c_4)J_2 \\ &\quad\; +(2c_3 - c_1)J_3 + (3c_4 - c_2)J_4, \quad c_k = (J_k, A). \end{aligned} \tag{2.9}$$

Try for $n = 5$. $\square$

Assume that the matrix $\mathcal{L}_A = \sum_{k=1}^m \alpha_k J_k$ is required in its explicit form, i.e. replace Problem 2.1 with

Problem 2.3 *Find the matrix $\mathcal{L}_A$ in $\mathcal{L} = Span\{J_1,\ J_2, \dots,\ J_m\}$ for which*

$$\|\mathcal{L}_A - A\|_F \leq \|X - A\|_F, \quad \forall X \in \mathcal{L}, \tag{2.10}$$

where A is any fixed $n \times n$ matrix.

If J'_k, $k = 1, \dots, m$, are m linearly independent matrices in $\mathcal{L}$, then one finds an alternative representation of $\mathcal{L}_A$:

$$\mathcal{L}_A \equiv \sum_{k=1}^m \alpha_k J_k = \sum_{k=1}^m \alpha'_k J'_k, \quad \alpha' = B'^{-1}\mathbf{c}', \quad c'_i = (J'_i, A), \;\; [B']_{i,j} = (J'_i, J'_j).$$

As a consequence, once the space $\mathcal{L}$ is fixed, one can try to look for a basis J_k of $\mathcal{L}$ for which the complexity of the inner products (J_i, A), $i = 1, \dots, m$, is minimal or, alternatively, for which the system $B\mathbf{z} = \mathbf{c}$ is easily solvable. The former requirement is in general satisfied by choosing J_k as sparse as possible. The latter requirement is fully satisfied by introducing an orthonormal basis of $\mathcal{L}$; in fact, if $B = I$, then $\alpha_k = c_k$ are the Fourier coefficients of A. Obviously one should be able to construct such orthonormal basis by a simple procedure, instead of utilizing the Gram-Schmidt algorithm.

If the J_k span an algebra $\mathcal{L}$ of group matrices, then the computation of the best least squares fit of A in $\mathcal{L}$ has minimal complexity. This is shown, in the following example, when $\mathcal{L} = \{\text{circulants}\}$.

Example 2. Let J_k be the $n \times n$ matrix

$$J_k = \frac{1}{\sqrt{n}} \begin{bmatrix} 0 & \cdots & \cdots & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & & & 0 & \ddots & \ddots & \vdots \\ \vdots & & & & & \ddots & 1 & 0 \\ 0 & & & & & & \ddots & 1 \\ 1 & 0 & & & & & & 0 \\ 0 & 1 & \ddots & & & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & & & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & 0 \end{bmatrix}$$

with $\mathbf{e}_1^T J_k = \mathbf{e}_k^T$. Notice that $\sqrt{n} J_k = (\sqrt{n} J_2)^{k-1}$, $\sqrt{n} J_1 = I$ and $J_n = J_2^T$. For any n one calculates $B = I$. Thus,

$$\mathcal{C}_A = \sum_{k=1}^{n} \alpha_k J_k = \sum_{k=1}^{n} c_k J_k, \quad c_k = (J_k, A). \tag{2.11}$$

Since the matrices J_k are sparse and orthonormal, the computation of the best least squares fit of A in the algebra $\mathcal{C} = \text{Span}\{J_1, \dots, J_n\}$ of *circulant* matrices has minimal complexity. For an exhaustive treatise on circulant matrices see [19]. $\square$

Notice, however, that circulants are not always the best approximations of A. In particular, if T is a symmetric Toeplitz matrix, then there exist two algebras, η and $\mathcal{H}$ (see [30], [9] and Section 3 of this paper), such that

$$\|\eta_T - T\|_F \leq \|\mathcal{H}_T - T\|_F \leq \|\mathcal{C}_T - T\|_F. \tag{2.12}$$

The algebra η does not have a simple sparse orthonormal basis as $\mathcal{C}$. However, if one needs to use the approximation $\mathcal{L}_T$ as a preconditioner of the Toeplitz linear system $T\mathbf{x} = \mathbf{b}$, a little more effort in computing $\mathcal{L}_T$ is widely justified by a better approximation level of T. In fact, the rate of convergence of the conjugate gradient method applied to $T\mathbf{x} = \mathbf{b}$ preconditioned by $\mathcal{L}_T$ will be intuitively greater for $\mathcal{L} = \eta$ than for $\mathcal{L} = \mathcal{C}$. A formula for η_T is obtained in [30]. The inequality (2.12), found in [30], also states that Hartley is not optimal for all values of n, thereby extending the remark of Figure 1 (regarding the case

$n = 3$). More details on the role of $\mathcal{L}_A$ in preconditioning techniques for linear systems $A\mathbf{x} = \mathbf{b}$ are reported in Section 3.

Best least squares fit in $\mathcal{L} \in \mathbb{V}$

When $\mathcal{L}$ is a space of matrices simultaneously diagonalized by a unitary transform U, some well known properties of $\mathcal{L}_A$, such as the fact that $\mathcal{L}_A$ inherites the positive definiteness from A, are shown in [43], [36], [41]. Now the same properties hold in the more general case where $\mathcal{L}$ has a suitable $\mathbb{V}$-structure [30] (see for example Theorem 2.6). This structure let us also obtain alternative representations of B (defined in (2.1)) especially useful in computing $\mathcal{L}_A$.

We say precisely that $\mathcal{L}$ is a $\mathbb{V}$ space (or $\mathcal{L}$ belongs to the class $\mathbb{V}$) if there exist a vector $\mathbf{v}$ and a basis $\{J_1,\ J_2, \ldots,\ J_n\}$ of $\mathcal{L}$ such that

$$\mathbf{v}^T J_k = \mathbf{e}_k^T. \tag{2.13}$$

A result proving that $\mathbb{V}$ represents a significant class of matrix spaces is the fact that a matrix X is nonderogatory iff the set of all polynomials in X is a space of class $\mathbb{V}$ [30].

Observe that two matrices A_1, A_2 of $\mathcal{L} \in \mathbb{V}$ for which $\mathbf{v}^T A_1 = \mathbf{v}^T A_2$, are equal. This is a sort of generalization of the assertion that two circulant matrices with the same first row are equal. The matrix $A = \sum_{k=1}^n z_k J_k$ is denoted by $\mathcal{L}_{\mathbf{v}}(\mathbf{z})$, and the row vector $\mathbf{v}^T A = \mathbf{z}^T = [z_1\ z_2 \cdots z_n]$ is called the $\mathbf{v}$-row of A. For $\mathbf{v} = \mathbf{e}_1$ simply set $\mathcal{L}(\mathbf{z}) = \mathcal{L}_{\mathbf{e}_1}(\mathbf{z})$; so $\mathcal{C}(\mathbf{z})$ denotes the circulant matrix with first row $\mathbf{z}^T$.

Problem 2: Given another basis J'_k of $\mathcal{L}$, is it possible to introduce a vector $\mathbf{v}'$ such that $\mathbf{v}'^T J'_k = \mathbf{e}_k^T$?

Lemma 2.4 *Assume that $\mathcal{L} \in \mathbb{V}$ is a matrix algebra, i.e. $J_i J_j \in \mathcal{L}, \forall i, j$, and $I \in \mathcal{L}$, where I is the identity matrix. If $A \in \mathcal{L}$ is invertible, then $A^{-1} = \mathcal{L}_{\mathbf{v}}(\mathbf{z})$, $\mathbf{z}^T A = \mathbf{v}^T$, i.e. $\mathcal{L}$ is closed under inversion.*

Proof. Let $\mathbf{z}$ be such that $\mathbf{z}^T A = \mathbf{v}^T$. Since $\mathbf{v}^T \mathcal{L}_{\mathbf{v}}(\mathbf{z}) A = \mathbf{v}^T I$, one has the equality $\mathcal{L}_{\mathbf{v}}(\mathbf{z}) A = I$. $\square$

Theorem 2.5 *Let $\mathcal{L}$ be a space of class $\mathbb{V}$ and let $\mathbf{v} \in \mathbb{C}^n$, $J_k \in \mathcal{L}$ satisfy* (2.13). *Let P_k be the $n \times n$ matrices defined by the identities $\mathbf{e}_k^T P_s = \mathbf{e}_s^T J_k$ and satisfying the equality $\sum v_k P_k = I$.*

Assume that $\mathcal{L}$ is a matrix algebra closed under conjugate transposition.

(i) We have

$$B = \sum_{k=1}^n (\mathrm{tr}\ J_k) \bar{P}_k. \tag{2.14}$$

(ii) If $v_k = \overline{\mathrm{tr}\ J_k}$, i.e.

$$[\ \overline{\mathrm{tr}\ J_1}\ \cdots\ \overline{\mathrm{tr}\ J_n}\ ] J_k = \mathbf{e}_k^T, \quad k = 1, \ldots, n, \tag{2.15}$$

then

$$\{J_k\} = \text{ orthonormal basis, i.e. } B = I. \tag{2.16}$$

(iii) If $\mathcal{L}$ is commutative, i.e. $J_iJ_j = J_jJ_i, \forall i,j$, then $J_k = P_k$ and

$$B = \sum_{k=1}^{n} (\mathrm{tr}\, J_k)\bar{J}_k, \tag{2.17}$$

so both $\bar{B}$ and $\bar{B}^{-1}$ are matrices of $\mathcal{L}$.

Proof. Exploit the definition of B to obtain the equality $[B]_{ij} = \sum_{r=1}^{n} [J_jJ_i^*]_{rr}$. The closure under conjugate transposition and under multiplication of $\mathcal{L}$ implies that $J_jJ_i^* = \sum_{k=1}^{n} a_kJ_k$ for some $a_k \in \mathbb{C}$. Finally, by condition (2.13), one has $a_k = [J_i^*]_{jk} = [\bar{P}_k]_{ij}$, and the representation of B in (2.14) is proved. Assertions (ii) and (iii) follow easily from assertion (i). $\square$

As it is shown in the following Example 3 in the case $\mathcal{L} = \tau$, the computation of $\alpha = B^{-1}\mathbf{c}$ can be simplified by using the information on B found in Theorem 2.5.

Example 3. In solving the exercise of Example 1, one observes that

$$B = \begin{bmatrix} 5 & 0 & 3 & 0 & 1 \\ 0 & 8 & 0 & 4 & 0 \\ 3 & 0 & 9 & 0 & 3 \\ 0 & 4 & 0 & 8 & 0 \\ 1 & 0 & 3 & 0 & 5 \end{bmatrix}, \quad B^{-1} = \frac{1}{12}\begin{bmatrix} 3 & 0 & -1 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 \\ -1 & 0 & 2 & 0 & -1 \\ 0 & -1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 & 3 \end{bmatrix}. \tag{2.18}$$

Theorem 2.5(iii) for $J_k = \tau(\mathbf{e}_k)$ together with (2.8) and (2.18) allows to deduce the explicit form of B and B^{-1} for generic values of n:

$$B = nJ_1 + (n-2)J_3 + \cdots + \begin{cases} J_n & n \text{ odd} \\ 2J_{n-1} & n \text{ even} \end{cases}, \quad B^{-1} = \frac{1}{2n+2}(3J_1 - J_3).$$

The inverse of B is obtained from the equality

$$\frac{1}{2n+2}[3\ 0\ -1\ 0\ \cdots\ 0]B = \mathbf{e}_1^T$$

and from Lemma 2.4. Thus an expression of τ_A for n generic is obtained:

$$\begin{aligned} \tau_A = \tfrac{1}{2n+2}\Big[&(3c_1 - c_3)J_1 + \textstyle\sum_{k=2}^{n-1}(2c_k - c_{k-2} - c_{k+2})J_k + \\ &(3c_n - c_{n-2})J_n\Big], \quad c_k = (J_k, A). \end{aligned} \tag{2.19}$$

$\square$

If the space $\mathcal{L}$ is such that there exist and can be easily computed matrices $J_k \in \mathcal{L}$ satisfying the condition (2.15), then $\mathcal{L}_A$ is simply given by its Fourier expansion

$$\mathcal{L}_A = \sum_{k=1}^{n} (J_k, A)J_k. \tag{2.20}$$

Example 4. The three matrices of the algebra τ

$$J_1 = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{bmatrix}, \quad J_2 = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix},$$
$$J_3 = \frac{1}{\sqrt{8}} \begin{bmatrix} -1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & -1 \end{bmatrix} \tag{2.21}$$

satisfy the identities

$$\mathbf{v}^T J_k = \mathbf{e}_k^T, \quad k = 1, 2, 3,$$

where $\mathbf{v}^T = [\mathrm{tr}\, J_1 \;\; \mathrm{tr}\, J_2 \;\; \mathrm{tr}\, J_3]$. So, by Theorem 2.5(ii), they define an orthonormal basis of τ. Thus, for $n = 3$, an expression of τ_A alternative to (2.19) holds:

$$\tau_A = (J_1, A)J_1 + (J_2, A)J_2 + (J_3, A)J_3, \quad J_k = \tau_{\mathbf{v}}(\mathbf{e}_k).$$

The matrices (2.21) can be obtained also by applying the Gram-Schmidt procedure to the three τ matrices

$$M_1 = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{bmatrix}, \quad M_2 = \begin{bmatrix} 2-z & 1-z & z \\ 1-z & 2 & 1-z \\ z & 1-z & 2-z \end{bmatrix},$$
$$M_3 = \begin{bmatrix} x+2y-4 & y & x \\ y & 2x+2y-4 & y \\ x & y & x+2y-4 \end{bmatrix}.$$

In fact,

$$\begin{aligned} &M_1 = \sqrt{8} J_1, \\ &M_2 - (J_1, M_2)J_1 = \sqrt{8} J_2, \\ &M_3 - (J_1, M_3)J_1 - (J_2, M_3)J_2 = \sqrt{8} J_3. \end{aligned}$$

□

Problem 3: Is it possible to define via (2.15) an orthonormal basis of τ for all n?

Problem 4: Under what assumptions on $\mathcal{L} \in \mathbb{V}$ there exist matrices J_k in $\mathcal{L}$ satisfying the conditions (2.15)?

The representation (2.17) of $B = ((J_i, J_j))_{i,j=1}^n$ holds under assumptions less restrictive than $J_i J_j = J_j J_i, \forall i, j$. Consider, in fact, a set $\{J_1, \; J_2, \ldots, \; J_n\}$ of linearly independent matrices (not necessarily spanning a $\mathbb{V}$ space). Then, by the definition of B,

$$[B]_{ij} = \sum_{r,s=1}^{n} \overline{[J_i]}_{rs} [J_j]_{rs} = \sum_{r,s=1}^{n} [J_i^*]_{sr} [J_j]_{rs} = \sum_{s=1}^{n} [J_i^* J_j]_{ss}.$$

Thus the identity $B = \sum_{k=1}^n (\mathrm{tr}\, J_k) \bar{J}_k$ holds iff $\mathrm{tr}(J_i^* J_j) = \mathrm{tr}\left(\sum_{k=1}^n \overline{[J_k]}_{i,j} J_k\right)$. In particular, the latter condition is satisfied if

$$J_i^* J_j = \sum_{k=1}^{n} \overline{[J_k]}_{i,j} J_k, \quad 1 \le i, j \le n. \tag{2.22*^{1}}$$

Now, ($2.22*^1$) together with the condition

$$I = \sum_{k=1}^{n} v_k J_k, \text{ for some } v_k \in \mathbb{C}, \tag{$2.22*^2$}$$

implies that $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $\mathbf{v} = [v_1\ v_2\ \cdots\ v_n]^T$, i.e. $\mathcal{L} = \text{Span}\{J_1, \dots, J_n\}$ is a member of $\mathbb{V}$. The following Theorem 2.6 proves that the conditions (2.22*), or, equivalently, the assumption $\mathcal{L}$=*space [30], imply several other properties on $\mathcal{L}$ and $\mathcal{L}_A$.

Theorem 2.6 *Assume that n linearly independent $n \times n$ matrices $J_1, \dots, J_n$ satisfy the conditions* (2.22*)*. Then the *space $\mathcal{L} = \text{Span}\{J_1,\ J_2, \dots,\ J_n\}$ has the following properties:*

(i) $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $k = 1, \dots, n$, where $\sum_{k=1}^n v_k J_k = I$; i.e. $\mathcal{L} \in \mathbb{V}$.
(ii) $\mathcal{L}$ is a matrix algebra.
(iii) $\mathcal{L}$ is closed under conjugate transposition.
Moreover, we have:
(iv) If $B = ((J_i, J_j))$, then

$$B = \sum_{k=1}^{n} (\text{tr } J_k) \bar{P}_k = \sum_{k=1}^{n} (\text{tr } J_k) \bar{J}_k \tag{2.23}$$

i.e. $\bar{B}$ and $\bar{B}^{-1}$ are in $\mathcal{L}$.
(v) If $c_k = (J_k, A)$ and $\mathbf{z} \in \mathbb{C}^n$, then $\mathbf{z}^* \mathcal{L}_{\mathbf{v}}(\mathbf{c}) \mathbf{z} = \sum_{k=1}^n [P_k^* \mathbf{z}]^* A [P_k^* \mathbf{z}]$.
(vi) If $A = A^*$, then $\mathcal{L}_A = \mathcal{L}_A{}^*$ and $\min \lambda(A) \le \lambda(\mathcal{L}_A) \le \max \lambda(A)$. In particular,

$$A \text{ hermitian positive definite } \Rightarrow \mathcal{L}_A \text{ hermitian positive definite .} \tag{2.24}$$

Proof. See [30]. □

Problem 5: Is it possible to extend the class of spaces $\mathcal{L}$ for which (2.24) holds? (Notice that $\mathcal{L}$ must be at least closed under conjugate transposition.)

Group matrix algebras represent an important class of *spaces. Before [30], it was known that if $\mathcal{L} = \mathcal{C} \equiv \{\text{circulants}\}$, then the matrix $\mathcal{L}_{T^TT}$, T =Toeplitz non singular, inherites positive definiteness from T^TT. Now, after [30], we know that this is true for any, commutative or non commutative, group matrix algebra $\mathcal{L}$. Moreover, the following example shows that computing $\mathcal{L}_{T^TT}$, $\mathcal{L} = \{\text{dihedral group matrices}\}$, is not more expensive than computing $\mathcal{C}_{T^TT}$.

Example 5 (Appendix notation). In the Appendix it is shown that if $T = (t_{i-j})_{i,j=0}^{n-1}$ is a generic Toeplitz matrix and $I(\mathbf{e}_r)$ is the Toeplitz matrix with $[I(\mathbf{e}_r)]_{0k} = \delta_{kr}$, $[I(\mathbf{e}_r)]_{k0} = 0$, then all inner products $(I(\mathbf{e}_r), T^TT)$, $(JI(\mathbf{e}_r), T^TT)$, $(I(\mathbf{e}_r)^T, T^TT)$, $(JI(\mathbf{e}_r)^T, T^TT)$, $r = 0, \dots, n-1$, where

$$J = \begin{bmatrix} 0 & \cdots & \cdots & 0 & 1 \\ \vdots & & \iddots & 1 & 0 \\ \vdots & \iddots & \iddots & \iddots & \vdots \\ 0 & 1 & \iddots & & \vdots \\ 1 & 0 & \cdots & \cdots & 0 \end{bmatrix}, \tag{2.25}$$

can be computed with $O(n \log n)$ arithmetic operations (see also [41]). As a consequence, the time complexity of the computation of the Fourier coefficients $c_k = (J_k, T^T T)$ in equality $\mathcal{C}_{T^T T} = \sum c_k J_k$, $J_k = \mathcal{C}(\frac{1}{\sqrt{n}}\mathbf{e}_k)$ (see (2.11)) is at most $O(n \log n)$. However, the same result holds in computing $c_k = (J_k, T^T T)$ in $\mathcal{D}_{T^T T} = \sum c_k J_k$, where $J_k = \mathcal{D}(\frac{1}{\sqrt{n}}\mathbf{e}_k)$ represent the obvious (orthonormal) basis of the dihedral group algebra

$$\mathcal{D} = \left\{ \begin{bmatrix} X & JY \\ JY & X \end{bmatrix} : X, Y \ \frac{n}{2} \times \frac{n}{2} \text{ circulants} \right\}.$$

The proof is based on the equality

$$T^T T = \begin{bmatrix} T_1^T T_1 + T_3^T T_3 & T_1^T T_2 + T_3^T T_1 \\ T_2^T T_1 + T_1^T T_3 & T_2^T T_2 + T_1^T T_1 \end{bmatrix},$$

where T_i are the $\frac{n}{2} \times \frac{n}{2}$ Toeplitz matrices defined by

$$T = \begin{bmatrix} T_1 & T_2 \\ T_3 & T_1 \end{bmatrix},$$

and on the remark that the matrices J_k can be written in terms of matrices $I(\mathbf{e}_r)$, $JI(\mathbf{e}_r)$, $I(\mathbf{e}_r)^T$, $JI(\mathbf{e}_r)^T$ of order n and $\frac{n}{2}$ (the details are left to the reader). $\square$

There is a class of *spaces which is associated with the set of the $n \times n$ unitary matrices. More precisely, if the $n \times n$ matrix U is such that $U^* = U^{-1}$, then the commutative matrix algebra

$$\mathcal{L} = sd\, U := \{U d(\mathbf{z}) U^* : \mathbf{z} \in \mathbb{C}\}, \quad d(\mathbf{z}) = \mathrm{diag}(z_1,\ z_2, \ldots,\ z_n),$$

is a *space, and thus all conclusions in Theorem 2.6 hold [30]. A collection of useful results on $\mathcal{L}_A$ and on its properties when $\mathcal{L} = sd\, U$, is given in the following

Theorem 2.7 *Let U be a $n \times n$ unitary matrix and let $\mathcal{L} = sd\, U$ be the space of all matrices simultaneously diagonalized by U. Let $\mathcal{L}_A = U d(\mathbf{z}_A) U^*$ denote the best l. s. fit to A in $\mathcal{L}$. Then*

(i) If $A = A^*$ then $\mathcal{L}_A = {\mathcal{L}_A}^*$ and

$$\min \lambda(A) \leq (\mathbf{z}_A)_i \leq \max \lambda(A)$$

*(ii) $\mathcal{L}_A$ is hermitian positive definite whenever A is hermitian positive definite. If, in particular, $\mathcal{L}$ is spanned by real matrices, then $\mathcal{L}_A$ is real symmetric positive definite (*pd*) whenever A is real symmetric positive definite (*pd*).*

(iii) $\mathcal{L}_A = U d(\mathbf{z}_A) U^*$, $(\mathbf{z}_A)_i = (U^* A U)_{ii}$, $i = 1, \ldots, n$.

(iv) $\mathbf{z}_{\mathbf{x}\mathbf{y}^T} = d(U^*\mathbf{x}) U^T \mathbf{y}$, $\mathbf{x},\ \mathbf{y} \in \mathbb{C}^n$.

(v) $\mathrm{tr}\, A = \mathrm{tr}\, \mathcal{L}_A$.

(vi) If A is hermitian positive definite, then $\det A \leq \det \mathcal{L}_A$.

Proof. The representation in (iii) is a simple consequence of the equality $\|U d(\mathbf{z}) U^* - A\|_F = \|d(\mathbf{z}) - U^* A U\|_F$. Notice that (i) and (ii) follows from Theorem 2.6 as well as from the $\mathcal{L}_A$ representation in (iii). Items (iv), (v) and (vi) follow from (iii). In particular, if A is hermitian positive definite, then, by the Hadamard inequality, we have

$$\det(\mathcal{L}_A) = \det d(\mathbf{z}_A) \geq \det(U^* A U) = \det(A).$$

□

A very useful representation of $\mathcal{L}_A$, $\mathcal{L} = sd\, U$, is obtained by exploiting the fact that $\mathcal{L}$ is in $\mathbb{V}$. In fact, for any $\mathbf{v} \in \mathbb{C}^n$ such that $[U^T\mathbf{v}]_i \neq 0$, $\forall i$, the matrices of the space $\mathcal{L}$ can be represented as

$$\mathcal{L}_{\mathbf{v}}(\mathbf{z}) = U d(U^T\mathbf{z}) d(U^T\mathbf{v})^{-1} U^*, \quad \mathbf{z} \in \mathbb{C}^n \tag{2.26}$$

(see Proposition 2.4 in [30]). So, given a vector $\mathbf{v} \in \mathbb{C}^n$ such that $[U^T\mathbf{v}]_i \neq 0\ \forall i$, if the $\mathbf{v}$-row of $\mathcal{L}_A$, i.e. $\mathbf{v}^T\mathcal{L}_A$, is given, then

$$\mathcal{L}_A = U d(U^T {\mathcal{L}_A}^T \mathbf{v}) d(U^T\mathbf{v})^{-1} U^* = U d(U^T B^{-1}\mathbf{c}) d(U^T\mathbf{v})^{-1} U^* \tag{2.27}$$

where the latter identity holds if the basis J_k of $\mathcal{L}$ is defined by $J_k = \mathcal{L}_{\mathbf{v}}(\mathbf{e}_k)$.

Example 6. At the beginning of the next Section 3 it is shown that the matrix algebras $\mathcal{C}$ and τ are $sd\, U$ spaces, i.e. satisfy the identities

$$\mathcal{C} = sd\, U_{\mathcal{C}}, \quad \tau = sd\, U_{\tau},$$

for suitable unitary matrices $U_{\mathcal{C}}$ and U_τ known as Fourier and sine transform, respectively. Thus the following representations of $\mathcal{C}_A$ and τ_A hold:

$$\mathcal{L}_A = U_{\mathcal{L}} d(U_{\mathcal{L}}^T B^{-1}\mathbf{c}) d(U_{\mathcal{L}}^T \mathbf{e}_0)^{-1} U_{\mathcal{L}}^*, \quad \mathcal{L} = \mathcal{C},\ \tau\ (J_k = \mathcal{L}(\mathbf{e}_k)) \tag{2.28}$$

(alternative to (2.11) and (2.19)) which let one reduce computations involving $\mathcal{C}_A$ and τ_A to *fast* Fourier and sine discrete transforms, respectively (computable in $O(n\log n)$ arithmetic operations). □

3 $\mathcal{L}_A$ as a Preconditioner ($A = T$, $A = T^T T$ where T is Toeplitz)

Because of the structure of transforms and related algebras involved in the present section, it is convenient to introduce a general setting for diagonal spaces $\mathcal{L}$ where one can retrieve the vector $\mathbf{z}$ defining the information sufficient to define a matrix $A \in \mathcal{L}$. This vector $\mathbf{z}$ is equal to a linear combination of the rows of A, that is $\mathbf{z}^T = \mathbf{v}^T A$, where for the most known algebras (circulant, τ, Hartley, Hessenberg) $\mathbf{v}^T = \mathbf{e}_0^T = [1\ 0 \cdots 0]$. To recall that a matrix $A \in \mathcal{L}$ is defined by $\mathbf{z}^T = \mathbf{v}^T A$ one can use the symbol $\mathcal{L}_{\mathbf{v}}(\mathbf{z})$ instead of A (see [30] or the previous section), and, in particular, the symbol $\mathcal{L}(\mathbf{z})$ if $\mathbf{v} = \mathbf{e}_0$. In order to follow the notation in [10], suitable for fast transforms, the indeces in this section and in the Appendix will run from 0 to $n-1$ (instead from 1 to n).

Let $U_{\mathcal{L}}$ be a unitary matrix and let $\mathcal{L}$ be the space of all matrices simultaneously diagonalized by $U_{\mathcal{L}}$, i.e. $\mathcal{L} = sd\, U_{\mathcal{L}} = \{U_{\mathcal{L}} d(\mathbf{z}) U_{\mathcal{L}}^* : \mathbf{z} \in \mathbb{C}^n\}$, $d(\mathbf{z}) = \operatorname{diag}(z_k, k = 0, \ldots, n-1)$. Choose a vector $\mathbf{v} \in \mathbb{C}^n$ so that the matrix

$$\mathcal{L}_{\mathbf{v}}(\mathbf{z}) = U_{\mathcal{L}} d(U_{\mathcal{L}}^T \mathbf{z}) d(U_{\mathcal{L}}^T \mathbf{v})^{-1} U_{\mathcal{L}}^* \tag{3.1}$$

is well defined. Notice that $\mathbf{v}^T\mathcal{L}_{\mathbf{v}}(\mathbf{z}) = \mathbf{z}^T$. Thus, any matrix A of $\mathcal{L}$ is determined by the vector $\mathbf{v}^T A$, the $\mathbf{v}$-row of A. If $\mathbf{v} = \mathbf{e}_0$, then $A \in \mathcal{L}$ is determined by its first row.

The formula (3.1) holds in particular for $\mathcal{L} = \mathcal{C}_{\pm 1}$ = the space of $n \times n$ (± 1)-circulant matrices. Any (± 1)-circulant matrix is determined by its first row $\mathbf{z}^T = [z_0\ z_1 \cdots z_{n-1}]^T$, $z_k \in \mathbb{C}$, via the formula

$$\mathcal{C}_{\pm 1}(\mathbf{z}) = \sum_{k=0}^{n-1} z_k P_{\pm 1}^k, \quad P_{\pm 1} = \begin{bmatrix} 0 & 1 & & \\ & & \ddots & \\ & & & 1 \\ \pm 1 & & & 0 \end{bmatrix}. \tag{3.2}$$

To see that $\mathcal{C}_{\pm 1}$ can be put in the form (3.1) set $\mathbf{v} = \mathbf{e}_0$, $U_{\mathcal{C}_1} = F$ and $U_{\mathcal{C}_{-1}} = DF$, where $D = \mathrm{diag}(e^{-\mathbf{i}j\pi/n}, j = 0, \ldots, n-1)$, $\mathbf{i} = \sqrt{-1}$, and F is the Fourier matrix

$$F = \frac{1}{\sqrt{n}}(e^{-\mathbf{i}2\pi ij/n})_{i,j=0}^{n-1}$$

(prove (3.1) first for $\mathbf{z} = \mathbf{e}_1$ and use (3.2)). Moreover, if $\mathcal{L}$ is the Jacobi algebra τ of Section 2, equivalently defined as the set of all matrices $X = (x_{ij})_{i,j=0}^{n-1}$ satisfying the cross-sum condition

$$x_{i-1,j} + x_{i+1,j} = x_{i,j-1} + x_{i,j+1} \tag{3.3}$$

with $x_{i,-1} = x_{-1,i} = x_{i,n} = x_{n,i} = 0$, then one can prove that (3.1) holds for $\mathbf{v} = \mathbf{e}_0$ and $U_\tau = \sqrt{\frac{2}{n+1}}(\sin\frac{(i+1)(j+1)\pi}{n+1})_{i,j=0}^{n-1}$.

Now let $\mathcal{C}_{\pm 1}^S$ and $\mathcal{C}_{\pm 1}^{SK}$ be, respectively, the spaces of all symmetric and skewsymmetric (± 1)-circulant matrices, i.e.

$$\mathcal{C}_{\pm 1}^S = \{X \in \mathcal{C}_{\pm 1} : X^T = X\}, \quad \mathcal{C}_{\pm 1}^{SK} = \{X \in \mathcal{C}_{\pm 1} : X^T = -X\},$$

and let $\mathrm{cas}\, x$ denote the function $\cos x + \sin x$. The Hartley matrix is defined by

$$H = \frac{1}{\sqrt{n}}\left(\mathrm{cas}\,\frac{2ij\pi}{n}\right)_{i,j=0}^{n-1}.$$

The discrete Hartley transform of a vector $\mathbf{z}$, $H\mathbf{z}$, is computable in $O(n\log n)$ arithmetic operations (a.o.), i.e. has the same computational complexity of the discrete Fourier transform $F\mathbf{z}$ (see [13], [45]). Note that $H = U_{\mathcal{H}}$ with $\mathcal{H} = \mathcal{C}_1^S + JP_1\mathcal{C}_1^{SK}$ where J is the reversal $n \times n$ matrix, i.e. $[J]_{ik} = \delta_{i,n-k-1}$ [9].

The matrix H can be naturally included in a set of eight *Hartley-type* (Ht) matrices [10]:

$$\begin{array}{llll} H, & HI_\eta^T, & K^T = \frac{1}{\sqrt{n}}(\mathrm{cas}\,\frac{(2i+1)j\pi}{n})_{i,j=0}^{n-1}, & K^T I_\eta, \\ K, & KI_\mu^T, & G = \frac{1}{\sqrt{n}}(\mathrm{cas}\,\frac{(2i+1)(2j+1)\pi}{2n})_{i,j=0}^{n-1}, & GI_\mu \end{array} \tag{3.4}$$

where

$$I_\eta = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{2} & & & \\ & I_{\lfloor\frac{n-1}{2}\rfloor} & & J_{\lfloor\frac{n-1}{2}\rfloor} \\ & & \sqrt{2} & \\ & -J_{\lfloor\frac{n-1}{2}\rfloor} & & I_{\lfloor\frac{n-1}{2}\rfloor} \end{bmatrix}, \quad I_\mu = \frac{1}{\sqrt{2}}\begin{bmatrix} I_{\lfloor\frac{n}{2}\rfloor} & & -J_{\lfloor\frac{n}{2}\rfloor} \\ & \sqrt{2} & \\ J_{\lfloor\frac{n}{2}\rfloor} & & I_{\lfloor\frac{n}{2}\rfloor} \end{bmatrix}.$$

In the above definitions I_k (J_k) is the identity (reversal) matrix of order k; moreover the presence of the central row and column including $\sqrt{2}$ depends on the oddness of n.

Each Ht transform can be reduced to a Hartley transform. In fact, if $R_{\mathcal{K}}$ and R_γ are the $n \times n$ symmetric orthogonal matrices

$R_{\mathcal{K}} = \mathrm{diag}(\cos\frac{\theta_k}{2}) + \mathrm{diag}(\sin\frac{\theta_k}{2})JP_1,$
$R_\gamma = \mathrm{diag}(\cos\frac{\varphi_k}{2}) + \mathrm{diag}(\sin\frac{\varphi_k}{2})J,$

where $\theta_k = \frac{2k\pi}{n}$, $\varphi_k = \frac{(2k+1)\pi}{n}$, $k = 0, \dots, n-1$, then

$$K^T = HR_{\mathcal{K}}, \quad G = R_\gamma K^T.$$

However, Ht radix-n_2 splitting formulas hold for *each* Ht transform $U = U_{n_1 n_2}$ and lead to factorizations of U_n, corresponding to factorizations of n, in terms of sparse orthogonal matrices [10]. The Ht radix-2 splitting formulas are reported in the following

Proposition 3.1 [10] *Let $Q_{n,2}$ be the even-odd (2-stride) permutation matrix defined by*

$$Q_{n,2}\mathbf{z} = [z_0\ z_2 \cdots z_{2n-2}\ z_1\ z_3 \cdots z_{2n-1}]^T, \quad \mathbf{z} \in \mathbb{C}^{2n}.$$

(i) For $U = H,\ K^T$, we have

$$U_{2n} = \frac{1}{\sqrt{2}} \begin{bmatrix} I & X \\ I & -X \end{bmatrix} \begin{bmatrix} U_n & 0 \\ 0 & U_n \end{bmatrix} Q_{n,2},$$

where $X = R_{\mathcal{K}}$ for $U = H$ and $X = R_\gamma$ for $U = K^T$.

(ii) Set

$R_\pm = \mathrm{diag}(\cos\frac{\varphi_k}{4}) \pm \mathrm{diag}(\sin\frac{\varphi_k}{4})J,$
$\tilde{R}_\pm = \mathrm{diag}(\cos\frac{\theta_k}{4}) \pm \mathrm{diag}(\sin\frac{\theta_k}{4})JP_{-1}.$

For $U = K,\ G$, we have

$$U_{2n} = \frac{1}{\sqrt{2}} \begin{bmatrix} X & Y \\ -YW & XW \end{bmatrix} \begin{bmatrix} U_n & 0 \\ 0 & U_n \end{bmatrix} Q_{n,2},$$

where $X = R_+$, $Y = R_-$, $W = J$ for $U = G$ and $X = \tilde{R}_+$, $Y = \tilde{R}_-$, $W = JP_{-1}$ for $U = K$.

The set of matrix algebras $\mathcal{L} = sd\, U_{\mathcal{L}}$, $U_{\mathcal{L}} = Ht$, can be also obtained:

$$\begin{array}{ll} \mathcal{H} = sd\, H = \mathcal{C}_1^S + JP_1\mathcal{C}_1^{SK}, & \alpha = sd\,(HI_\eta^T) = \mathcal{C}_1^S + JP_1\mathcal{C}_1^S, \\ \delta = sd\, K^T = \mathcal{C}_1^S + J\mathcal{C}_1^{SK}, & \eta = sd\,(K^T I_\eta) = \mathcal{C}_1^S + J\mathcal{C}_1^S, \\ & \\ \mathcal{K} = sd\, K = \mathcal{C}_{-1}^S + JP_{-1}\mathcal{C}_{-1}^{SK}, & \beta = sd\,(KI_\mu^T) = \mathcal{C}_{-1}^S + JP_{-1}\mathcal{C}_{-1}^S, \\ \gamma = sd\, G = \mathcal{C}_{-1}^S + J\mathcal{C}_{-1}^{SK}, & \mu = sd\,(GI_\mu) = \mathcal{C}_{-1}^S + J\mathcal{C}_{-1}^S. \end{array} \tag{3.5}$$

Notice that the equality (3.1) holds for γ with $\mathbf{v} \neq \mathbf{e}_0$ [30] since the condition $[G^T\mathbf{e}_0]_i \neq 0$, $\forall i$, is not verified in general.

The algebras $\mathcal{H}$, α, δ, η, $\mathcal{K}$, β, γ, μ represent the Ht counterpart of the set of eight Jacobi algebras (including τ) considered in [38]. However matrices from Jacobi algebras are polynomials in a symmetric tridiagonal matrix, whereas no simple nonderogatory matrix generating Ht is known [23], [10]. The algebras listed in (3.5) can have different effects in a number of applications, including displacement decompositions, preconditioning techniques and newtonian algorithms for unconstrained minimization. Some Ht algebras have been used in displacement and Bezoutian theory, i.e. as the factors M_i, N_i in matrix representations $A = \sum M_i N_i$ [23], [4], [22], [33], [34]. For A equal to the inverse of a Toeplitz-plus-Hankel ($T + H$) matrix, the latter representations are the basis of efficient direct $T + H$ linear systems solvers. In [33], [34] the matrices H, K, K^T and G are named H^I, H^{II}, H^{III} and H^{IV}, respectively, and are used to represent Toeplitz-plus-Hankel Bezoutians. The $\mathcal{L}QN$ minimization methods, recently introduced in [25], have been initially implemented for $\mathcal{L} = \mathcal{H}$ =Hartley algebra [26], [11]. Notice that the four Ht transforms H, K, K^T and G have been introduced independently in [35].

The Ht algebras $\mathcal{H}$ and $\mathcal{K}$, η, μ have been exploited in [9], [37] and in [30], respectively, to define preconditioners in solving positive definite Toeplitz systems $T\mathbf{x} = \mathbf{b}$, $T = (t_{|i-j|})_{i,j=0}^{n-1}$, by the conjugate gradient (CG) method. It has been noticed that such preconditioners, which are the best l.s. fits $\mathcal{H}_T$, $\mathcal{K}_T$, η_T and μ_T, approximate T better than the T.Chan-Huckle fit $(\mathcal{C}_{\pm 1})_T$ [18], [36]. In fact, the latter matrix, $(\mathcal{C}_{\pm 1})_T$, is a symmetric (± 1)-circulant matrix and Ht includes, by definition, symmetric (± 1)-circulant matrices. Moreover, among Ht, η and μ yield the best approximations of T [30]. The latter remark is essentially based on the fact that η and μ are the only Ht algebras which are simultaneously symmetric and persymmetric like T. So, one obtains the inequalities (2.12) ($\mathcal{C} = \mathcal{C}_1$) and

$$\|\mu_T - T\|_F \leq \|\mathcal{K}_T - T\|_F \leq \|(\mathcal{C}_{-1})_T - T\|_F \tag{3.6}$$

which justify the use of Ht matrices as preconditioners.

The following theorem reports explicit formulas for $(\mathcal{C}_{-1})_T$, $\mathcal{K}_T$ and μ_T (n even), and states that, at least for a class of positive definite Toeplitz matrices T, the eigenvalues of $\mathcal{L}_T^{-1}T$, $\mathcal{L} = \mathcal{C}_{-1}, \mathcal{K}, \mu$, are *clustered* around 1. It follows (see [1], [2]) that such matrices $\mathcal{L}_T$ can be efficiently used as preconditioners of $T\mathbf{x} = \mathbf{b}$. Analogous results hold for $\mathcal{L} = \mathcal{C}$ [16], $\mathcal{L} = \mathcal{H}$ [9], $\mathcal{L} = \eta$ [30].

Theorem 3.2 [30] *a) Let $T = (t_{|i-j|})_{i,j=0}^{n-1}$ be a symmetric Toeplitz matrix. Set $s_i = t_i + t_{n-i}$, $i = 0, \dots, n-1$ ($t_n = -t_0$), and $a_i = t_i - \frac{i}{n}s_i$, $i = 0, 1, \dots, n-1$. Notice that $s_i = s_{n-i}$, $a_{n-i} = -a_i$. Moreover, if n is even, set*

$$\begin{array}{ll} b_{2k} = \frac{2}{n}\left(\sum_{j=k+1}^{\lfloor \frac{n}{4} \rfloor} s_{2j-1} + t_{n/2}\delta_{n/2,o}\right), & k = 0, 1, \dots, \lfloor \frac{n}{4} \rfloor, \\ b_{2k-1} = \frac{2}{n}\left(\sum_{j=k}^{\lceil \frac{n}{4} \rceil - 1} s_{2j} + t_{n/2}\delta_{n/2,e}\right), & k = 1, \dots, \lceil \frac{n}{4} \rceil, \\ b_{n-j} = -b_j, & j = 1, \dots, \frac{n}{2} - 1, \frac{n}{2} \end{array}$$

where $\delta_{n/2,e(o)} = 1$, if $n/2$ is even (odd), and $\delta_{n/2,e(o)} = 0$, if $n/2$ is odd (even). Then

$$\mathcal{L}_T = U_{\mathcal{L}} d(U_{\mathcal{L}}^T \mathbf{z}) d(U_{\mathcal{L}}^T \mathbf{e}_0)^{-1} U_{\mathcal{L}}^* \tag{3.7}$$

where, for $i = 0, \dots, n-1$,

$$z_i = \begin{cases} a_i & \mathcal{L} = \mathcal{C}_{-1} \\ a_i + \frac{s_i}{n} & \mathcal{L} = \mathcal{K} \\ a_i + b_{n-i-1} & \mathcal{L} = \mu,\ n \text{ even.} \end{cases}$$

b) If $\{t_j\}_{j=0}^{+\infty}$ is a sequence of real numbers satisfying $\sum |t_j| < +\infty$ and $T^{(n)}$ is the Toeplitz matrix $T^{(n)} = (t_{|i-j|})_{i,j=0}^{n-1}$, then the eigenvalues of $\mathcal{L}_{T^{(n)}} - T^{(n)}$, $\mathcal{L} = \mathcal{C}_{-1}$, $\mathcal{K}$, μ, are clustered around zero, i.e. for any fixed ε, $\exists\ k_\varepsilon$ and ν_ε, $\nu_\varepsilon \geq k_\varepsilon$, such that $\forall n > \nu_\varepsilon$ at least $n - k_\varepsilon$ eigenvalues of $\mathcal{L}_{T^{(n)}} - T^{(n)}$ are in the interval $(-\varepsilon, \varepsilon)$.

Moreover, if $\sum t_{|j|} e^{\mathbf{i}j\theta} > 0$, $\forall \theta \in [-\pi, \pi]$, then $T^{(n)}$ and $\mathcal{L}_{T^{(n)}}$ are pd, and the eigenvalues of $I - \mathcal{L}_{T^{(n)}}{}^{-1} T^{(n)}$ are clustered around zero.

In the remaining part of this section $\mathcal{L}_A$, $\mathcal{L} = Ht$, is proposed as a preconditioner of CG in the case of non symmetric Toeplitz linear systems.

A way to solve the linear system

$$T\mathbf{x} = \mathbf{b}, \quad \det T \neq 0,$$

where T is a generic (possibly nonsymmetric) $n \times n$ real Toeplitz matrix $T = (t_{i-j})_{i,j=0}^{n-1}$ and $\mathbf{b} \in \mathbb{R}^n$, is to apply the CG method to the normal equations $T^T T\mathbf{x} = T^T\mathbf{b}$ or, more generally, to the *preconditioned* system

$$(TE^{-T})^T (TE^{-T})\mathbf{y} = (TE^{-T})^T\ \mathbf{b}, \quad E^T\mathbf{x} = \mathbf{y} \tag{3.8}$$

where E is a nonsingular matrix.

The CG method applied to (3.8) will be called CGP method, with P denoting the preconditioning matrix EE^T. In fact, the coefficient matrix in the system (3.8) is similar to $P^{-1}T^T T$ for any E such that $EE^T = P$. Thus it is the choice of P that influences the distribution of the eigenvalues of $E^{-1}T^T TE^{-T} = (TE^{-T})^T(TE^{-T})$ and therefore the rate of convergence of CG applied to (3.8) [1], [2], [16], [30].

At each step the CGP method requires two matrix vector products, $T\mathbf{z}$ and $T^T\mathbf{w}$ (besides a small number of inner products of complexity $O(n)$). These computations can be performed with $O(n \log n)$ a.o., either by using the identities

$$\begin{bmatrix} T\mathbf{z} \\ \mathbf{z}' \end{bmatrix} = \mathcal{C}(\mathbf{t}) \begin{bmatrix} \mathbf{z} \\ \mathbf{0} \end{bmatrix} = \sqrt{2n}\hat{F} d(\hat{F}\mathbf{t})\hat{F}^* \begin{bmatrix} \mathbf{z} \\ \mathbf{0} \end{bmatrix},$$
$$\begin{bmatrix} T^T\mathbf{w} \\ \mathbf{w}' \end{bmatrix} = \mathcal{C}(\mathbf{t})^T \begin{bmatrix} \mathbf{w} \\ \mathbf{0} \end{bmatrix} = \sqrt{2n}\hat{F} d(\hat{J}\hat{P}_1\hat{F}\mathbf{t})\hat{F}^* \begin{bmatrix} \mathbf{w} \\ \mathbf{0} \end{bmatrix},$$

where $\mathcal{C}(\mathbf{t})$ is the circulant matrix with first row $\mathbf{t}^T = [t_0\ t_{-1} \cdots t_{-n+1}\ 0\ t_{n-1} \cdots t_1]$ and $\hat{F}$, $\hat{J}$, $\hat{P}_1$ are the Fourier, the J and the P_1 matrices of dimension $2n$ (see (2.25) and (3.2)), or by using the procedures in [41], [32], [38] in terms of real transforms only. Moreover, in CGP a system $P\mathbf{z} = \mathbf{w}$ needs to be solved.

Clearly CGP is well defined and more efficient than CG applied to the linear system $T^T T\mathbf{x} = T^T\mathbf{b}$ (which is in general outperformed by direct methods, having a slow rate of convergence) provided that

1. P is pd (i.e. real symmetric positive definite);
2. P is computable in at most $O(n \log n)$ a.o.;
3. $P\mathbf{z} = \mathbf{w}$ is solvable in at most $O(n \log n)$ a.o.;
4. the spectrum of $P^{-1}T^TT$ is more "clustered" than the spectrum of T^TT.

Intuitively, in order to obtain the property 4, the matrix P should be a good approximation of T^TT. In this section $P = \mathcal{L}_{T^TT}$, i.e. P is the best least squares fit to T^TT from suitable subspaces $\mathcal{L}$ of $\mathbb{C}^{n\times n}$. This choice of P is suggested in [41] in the case $\mathcal{L}$ is a Jacobi matrix algebra. The matrix $\mathcal{L}_{T^TT}$ is also studied in [14] for $\mathcal{L} = \mathcal{C} \equiv \mathcal{C}_1 \equiv \{n \times n \text{ circulants}\}$. Here $\mathcal{L}_{T^TT}$ is shown to satisfy the conditions 1,2,3 for five different Ht matrix algebras $\mathcal{L}$. However, by the same definition of Ht in terms of $\mathcal{C}^S_{\pm 1}$ and $\mathcal{C}^{SK}_{\pm 1}$, it will be clear that the latter result can be extended to all eight Ht. Involving Ht instead of $\mathcal{C}_{\pm 1}$ is clearly justified since Ht approximate T^TT better than (± 1)-circulants. In fact, because $(\mathcal{C}_{\pm 1})_{T^TT} \in \mathcal{C}^S_{\pm 1}$, we have

$$
\begin{aligned}
\|\mathcal{L}_{T^TT} - T^TT\|_F &\le \|(\mathcal{C}_1)_{T^TT} - T^TT\|_F, \quad \mathcal{L} = \mathcal{H}, \alpha, \delta, \eta, \\
\|\mathcal{L}_{T^TT} - T^TT\|_F &\le \|(\mathcal{C}_{-1})_{T^TT} - T^TT\|_F, \quad \mathcal{L} = \mathcal{K}, \beta, \gamma, \mu.
\end{aligned}
\tag{3.9}
$$

Regarding condition 4, some numerical experiences in Table 1 prove that $CG(Ht)_{T^TT}$ outperforms the $CG(I_{T^TT})$ method and is competitive with $CG(\mathcal{L}_{T^TT})$ where $\mathcal{L}$ is one of the more widely exploited algebras $\mathcal{C}$, $\mathcal{C}_{-1}$ and the Jacobi τ. Moreover, the general framework here considered allows us to conclude that the conditions 1,2,3 hold also for spaces $\mathcal{L}$ of matrices which are not simultaneously diagonalized by a unitary matrix. The latter result is shown in detail in Example 5 of Section 2 when $\mathcal{L}$ is the (non commutative) dihedral group algebra $\mathcal{D}$. Some related numerical experiments show the efficiency of $\mathcal{D}$ as preconditioner even for matrices whose structure is not so close to the four–block dihedral frame.

Remark. In [17], [15] the choice $P = \mathcal{C}_T^T\mathcal{C}_T$ ($E = \mathcal{C}_T^T$) is suggested, where $\mathcal{C}_T$ is the best l.s. fit to T from the space of circulant matrices $\mathcal{C}$:

$$
\mathcal{C}_T = \frac{1}{n}\sum_{k=0}^{n-1}[(n-k)t_{-k} + kt_{n-k}]P_1^k.
$$

However, for both Jacobi and Ht matrix algebras $\mathcal{L}$ the choice $P = {\mathcal{L}_T}^T\mathcal{L}_T$ is not recommended since $\mathcal{L}_T$ is symmetric, even if T is not (for the Jacobi case see [41]). $\square$

Let us restrict the attention to spaces $\mathcal{L} = sd\, U_{\mathcal{L}}$, where $U_{\mathcal{L}}$ defines a transform computable in $O(n \log n)$ a.o.. Examples of such spaces are $\mathcal{C}_{\pm 1}$, Jacobi [46] and Ht. By Theorem 2.7(ii), the condition 1 is satisfied for $P = \mathcal{L}_{T^TT}$, $\mathcal{L} = \mathcal{C}_{\pm 1}, \text{Jacobi}, Ht$. The conditions 2 and 3 are satisfied for $P = \mathcal{L}_{T^TT}$ provided that the vector $\mathbf{a}$ in the equality $\mathcal{L}_{T^TT} = U_{\mathcal{L}} d(\mathbf{a}) U^*_{\mathcal{L}}$ is computable in at most $O(n \log n)$ a.o.. The fast computation of $\mathbf{a}$ is shown by Potts and Steidl [41] in the Jacobi case. Here we extend the result to the Ht case and give *explicit* formulas for $\mathbf{a}$. To this aim an expression for the vector $\mathbf{a}$ more convenient than $\mathbf{a} = ([U^*_{\mathcal{L}} T^TTU_{\mathcal{L}}]_{kk})_{k=0}^{n-1}$ (see Theorem 2.7(iii)) is needed.

Recall that if A is a generic $n \times n$ matrix, $\mathbf{v} \in \mathbb{C}^n$ is such that $[U_{\mathcal{L}}^T \mathbf{v}]_i \neq 0$, $\forall i$, and $J_k = \mathcal{L}_{\mathbf{v}}(\mathbf{e}_k)$, $\mathcal{L} = sd\, U_{\mathcal{L}}$, then

$$\mathcal{L}_A = U_{\mathcal{L}} d(\mathbf{a}) U_{\mathcal{L}}^*, \quad \mathbf{a} = d(U_{\mathcal{L}}^T \mathbf{v})^{-1} U_{\mathcal{L}}^T B^{-1} \mathbf{c}. \tag{3.10}$$

In the following we give procedures for the computation of $B^{-1}\mathbf{c}$ in (3.10) in the cases $\mathcal{L} = \eta$, $\mathbf{v} = \mathbf{e}_0$, and $\mathcal{L} = \gamma$, $\mathbf{v} = \mathbf{e}_0 + \mathbf{e}_{n-1}$. The latter choice of $\mathbf{v}$ is justified by the fact that $A \in \gamma$ is always determined by its $\mathbf{e}_0 + \mathbf{e}_{n-1}$-row ($[U_\gamma^T(\mathbf{e}_0 + \mathbf{e}_{n-1})]_i \neq 0$, $\forall i$), whereas there are values of n for which $\mathbf{e}_0^T A$, $A \in \gamma$, does not define A (some entries $[U_\gamma^T \mathbf{e}_0]_i = [G^T \mathbf{e}_0]_i$ are zero for $n = 6 + 4r$). We also give explicit formulas for $B^{-1}\mathbf{c}$, $\mathcal{L} \in \{\mathcal{C}_{\pm 1}, \mathcal{H}, \mathcal{K}, \eta, \mu\}$, $J_k = \mathcal{L}(\mathbf{e}_k)$. *The above procedures and formulas can be implemented in $O(n)$ a.o., provided that a fixed set of vectors $\mathbf{r}_A$, $\tilde{\mathbf{r}}_A$, $\mathbf{h}_A$, $\tilde{\mathbf{h}}_A$ is known.* The components of such vectors are the inner products

$$\begin{array}{ll} r_{k,A} = (I(\mathbf{e}_k), A), & \tilde{r}_{k,A} = (I(\mathbf{e}_k)^T, A), \\ h_{k,A} = (JI(\mathbf{e}_{n-1-k})^T, A), & \tilde{h}_{k,A} = (JI(\mathbf{e}_{n-1-k}), A), \end{array} \tag{3.11}$$

$k = 0, \dots, n-1$, where $I(\mathbf{z})$ is the upper triangular Toeplitz matrix with first row $\mathbf{z}^T$

$$I(\mathbf{z}) = \begin{bmatrix} z_0 & z_1 & \cdots & z_{n-1} \\ 0 & z_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & z_1 \\ 0 & \cdots & 0 & z_0 \end{bmatrix} \tag{3.12}$$

($I(\mathbf{e}_n) = 0$). Observe that

$$\mathbf{r}_A = \tilde{\mathbf{r}}_{JAJ} = \tilde{\mathbf{r}}_{A^T}, \quad \tilde{\mathbf{r}}_{JA} = J\mathbf{h}_A, \quad \mathbf{h}_A = \tilde{\mathbf{h}}_{JAJ} = \tilde{\mathbf{h}}_{JA^TJ}. \tag{3.13}$$

If A is generic, one needs to perform $O(n^2)$ a.o. in order to compute the components in (3.11). However, by Lemma 5.1 in the Appendix, if $A = T^T T$ where T is Toeplitz, then $\mathbf{r}_A$, $\tilde{\mathbf{r}}_A$, $\mathbf{h}_A$, $\tilde{\mathbf{h}}_A$ are computable in $O(n \log n)$ a.o.. So, one obtains the next Theorems 3.3, 3.5, and Corollary 3.8.

Computing η_A

Theorem 3.3 *The vector $\mathbf{a} = d(U_\eta^T \mathbf{e}_0)^{-1} U_\eta^T B^{-1} \mathbf{c}$ in the equality $\eta_A = U_\eta d(\mathbf{a}) U_\eta^*$, $\eta = \mathcal{C}_1^S + J\mathcal{C}_1^S$, $A = T^T T$, is computable in at most $O(n \log n)$ a.o.. So, the conditions 1, 2, 3 on preconditioners P of $T^T T$ are satisfied for $P = \eta_{T^T T}$.*

Let us give a procedure for the computation of $B^{-1}\mathbf{c}$, $J_k = \eta(\mathbf{e}_k)$. The matrix B^{-1} was computed in [30] by using the remark that $B^{-1} \in \eta$ (Theorem 2.6(iv)). In fact, if

$$T_{0,0}^{\pm 1, \pm 1} = \begin{bmatrix} 0 & 1 & & & \pm 1 \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 0 & 1 \\ \pm 1 & & & 1 & 0 \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}, \quad \mathbf{o} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, \tag{3.14}$$

and B denotes the matrix $((\mathcal{L}(\mathbf{e}_i), \mathcal{L}(\mathbf{e}_j)))_{i,j=0}^{n-1}$, $\mathcal{L} \in \{\eta, \mu\}$, then

$$B^{-1} = \frac{1}{2n}\left(2I \pm JT_{0,0}^{\pm 1,\pm 1}\right) - \frac{1}{n^2}\left[\mathbf{e}\mathbf{e}^T + \mathbf{o}\mathbf{o}^T \pm J(\mathbf{e}\mathbf{o}^T + \mathbf{o}\mathbf{e}^T)\right] \tag{3.15}$$

where the upper and lower signs refer, respectively, to the cases $\mathcal{L} = \eta$ and $\mathcal{L} = \mu$ [30]. The matrix vector product $B^{-1} \cdot \mathbf{c}$ can be clearly calculated in $O(n)$ a.o.. Thus, Theorem 3.3 is proved if the vector $\mathbf{c}$ is computable in $O(n \log n)$ a.o. for $A = T^T T$.

A direct computation of $\mathbf{c} = ((J_k, T^T T))_{k=0}^{n-1}$ is not recommended because the matrices $J_k = \eta(\mathbf{e}_k)$ are not sparse. For example, by using the cross-sum conditions (3.3) with $x_{-1,n-1-k} = x_{k,n} = x_{n,k} = x_{n-1-k,-1} = x_{0,k}$ (satisfied by any η matrix X [30]), one can write $\eta(\mathbf{e}_{\frac{n}{4}})$ and realize that it has $\frac{n^2}{4}$ nonzero entries. In Lemma 3.4 we introduce a basis $\{J_k'\}$ of $\eta = \mathcal{C}_1^S + J\mathcal{C}_1^S$ where each matrix J_k' can be written in terms of a constant number of matrices $I(\mathbf{e}_k)$, $I(\mathbf{e}_k)^T$, $JI(\mathbf{e}_{n-1-k})^T$, $JI(\mathbf{e}_{n-1-k})$. The basis $\{J_k'\}$ is obtained by grouping together the obvious basis of $\mathcal{C}_1^S$ and $J\mathcal{C}_1^S$ and by omitting the surplus. As a consequence, by Lemma 5.1 of Appendix, the vector $\mathbf{c}' = ((J_k', T^T T))_{k=0}^{n-1}$ is computable in $O(n \log n)$ a.o.. The next Lemma 3.4 also provides some relations between $\{J_k'\}$ and $\{J_k\}$ which imply that $\mathbf{c}$ is computable from $\mathbf{c}'$ in $O(n)$ a.o.. So, Theorem 3.3 is proved.

For $k = 0, 1, \ldots, n$ set

$$Z_k = I(\mathbf{e}_k) + I(\mathbf{e}_k)^T + I(\mathbf{e}_{n-k}) + I(\mathbf{e}_{n-k})^T \tag{3.16}$$

$(I(\mathbf{e}_n) = 0)$. Notice that $Z_0 = 2I$, $Z_1 = T_{0,0}^{1,1}$, $Z_j = Z_{j-1}Z_1 - Z_{j-2}$, $j = 2, \ldots, n$. Moreover, the set $\{A_k\}_{k=0}^{\lfloor \frac{n}{2} \rfloor}$, $A_0 = \frac{1}{2}Z_0 = \frac{1}{2}Z_n$, $A_k = Z_k = Z_{n-k}$, $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$, $A_{\frac{n}{2}} = \frac{1}{2}Z_{\frac{n}{2}}$ (n even), is the obvious basis of $\mathcal{C}_1^S$.

Lemma 3.4 [31] *The set of $n \times n$ matrices $\{J_k'\}$ where*

$$J_k' = \begin{cases} A_k & 0 \le k \le \lfloor \frac{n}{2} \rfloor \\ JA_{k-\lfloor \frac{n}{2} \rfloor - 1} & \lfloor \frac{n}{2} \rfloor + 1 \le k \le n-1 \end{cases} \tag{3.17}$$

form a basis of η. Moreover the basis $\{J_k\}$, $J_k = \eta(\mathbf{e}_k)$, can be expressed in terms of the J_k' by the following identities:

$$J_k = \begin{cases} J_0' = I & k = 0 \\ J_{k-2} + J_k' - J_{k+\lfloor \frac{n}{2} \rfloor}' & 1 \le k \le \lfloor \frac{n-1}{2} \rfloor \ (J_{-1} = 0) \\ J_k' & k = \frac{n}{2} \ (n \text{ even}) \\ -J_{n-k} + J_{n-k}' & \lfloor \frac{n}{2} \rfloor + 1 \le k \le n-1. \end{cases} \tag{3.18}$$

Thus, for the vectors $\mathbf{c} = ((J_k, A))_{k=0}^{n-1}$ and $\mathbf{c}' = ((J_k', A))_{k=0}^{n-1}$ we have

$$c_k = \begin{cases} c_0' = \operatorname{tr} A & k = 0 \\ c_{k-2} + c_k' - c_{k+\lfloor \frac{n}{2} \rfloor}' & 1 \le k \le \lfloor \frac{n-1}{2} \rfloor \ (c_{-1} = 0) \\ c_k' & k = \frac{n}{2} \ (n \text{ even}) \\ -c_{n-k} + c_{n-k}' & \lfloor \frac{n}{2} \rfloor + 1 \le k \le n-1. \end{cases} \tag{3.19}$$

Proof. The set $\mathcal{S} = \{A_k, JA_k : k = 0, \dots, \lfloor \frac{n}{2} \rfloor\}$ generates η. Let n be odd. Since $[\sum_{k=0}^{\frac{n-1}{2}} A_k]_{ij} = 1$, $\forall i, j$, we have $\sum_{k=0}^{\frac{n-1}{2}} JA_k = \sum_{k=0}^{\frac{n-1}{2}} A_k$ and thus $JA_{\frac{n-1}{2}}$ is a linear combination of the remaining matrices in $\mathcal{S}$. Analogously, if n is even, the identity $J(\sum_{k=0,k\ even}^{\frac{n}{2}} A_k) = \sum_{k=0,k\ odd}^{\frac{n}{2}} A_k$ implies that $JA_{\frac{n}{2}}$ and $JA_{\frac{n}{2}-1}$ are linear combinations of the other matrices in $\mathcal{S}$. In order to prove (3.18), it is sufficient to verify that the first row of the matrices on the right hand-side are the vectors $\mathbf{e}_k^T$, $0 \le k \le n-1$. $\square$

Proof of Theorem 3.3 (in detail). The vector $\mathbf{a}$ in the equality $\eta_{T^T T} = U_\eta d(\mathbf{a}) U_\eta^T$ is computable in $O(n \log n)$ a.o. by the following steps. Calculate the inner products vectors $\tilde{\mathbf{r}}_{T^T T} = \mathbf{r}_{T^T T}$, $\mathbf{h}_{T^T T}$ and $\tilde{\mathbf{h}}_{T^T T} = \mathbf{h}_{T T^T}$ by using formulas (5.1) and (5.2) in the Appendix. For $A = T^T T$ set

$$c'_k = \begin{cases} r_{0,A} & k = 0 \\ 2(r_{k,A} + r_{n-k,A}) & 1 \le k \le \lfloor \frac{n-1}{2} \rfloor \\ 2r_{\frac{n}{2},A} & k = \frac{n}{2}\ (n \text{ even}) \\ h_{n-1,A} = \tilde{h}_{n-1,A} & k = \lfloor \frac{n}{2} \rfloor + 1 \\ h_{n-k+\lfloor \frac{n}{2} \rfloor,A} + \tilde{h}_{n-k+\lfloor \frac{n}{2} \rfloor,A} + & \\ \qquad h_{k-\lfloor \frac{n}{2} \rfloor -2,A} + \tilde{h}_{k-\lfloor \frac{n}{2} \rfloor -2,A} & \lfloor \frac{n}{2} \rfloor + 2 \le k \le n-1. \end{cases} \tag{3.20}$$

Calculate $\mathbf{c}$ from $\mathbf{c}'$ and then $\mathbf{z}_\eta = B^{-1}\mathbf{c}$ by using, respectively, (3.19) and (3.14), (3.15). Then $\mathbf{a} = d(U_\eta^T \mathbf{e}_0)^{-1} U_\eta^T \mathbf{z}_\eta$. $\square$

Computing γ_A

Theorem 3.5 *The vector* $\mathbf{a} = d(U_\gamma^T(\mathbf{e}_0 + \mathbf{e}_{n-1}))^{-1} U_\gamma^T B^{-1}\mathbf{c}$ *in the equality* $\gamma_{T^T T} = U_\gamma d(\mathbf{a}) U_\gamma^*$, $\gamma = \mathcal{C}_{-1}^S + J\mathcal{C}_{-1}^{SK}$, *is computable in at most* $O(n \log n)$ *a.o.. So, the conditions 1, 2, 3 on preconditioners* P *of* $T^T T$ *are satisfied for* $P = \gamma_{T^T T}$.

Let us give a procedure for the computation of $B^{-1}\mathbf{c}$, $J_k = \gamma_{\mathbf{e}_0+\mathbf{e}_{n-1}}(\mathbf{e}_k)$. Since the matrices J_k are dense and $\forall n$ have not a simple explicit structure, a direct computation of B^{-1} and $\mathbf{c}$ is not recommended. However, the existence of J_k allows us to obtain a simple expression of $B^{-1}\mathbf{c}$ in terms of a suitable vector $B'^{-1}\mathbf{c}'$ where B'^{-1}, $\mathbf{c}'$ and $B'^{-1} \cdot \mathbf{c}'$ are easily computable.

Lemma 3.6 *The set of* $n \times n$ *matrices* $\{J'_k\}$ *where*

$$J'_k = \begin{cases} I & k = 0 \\ \mathcal{C}_{-1}(\mathbf{e}_k - \mathbf{e}_{n-k}) & 1 \le k \le \lceil \frac{n}{2} \rceil - 1, \end{cases} \tag{3.21^1}$$

$$J'_{\lceil \frac{n}{2} \rceil + k} = \begin{cases} J\mathcal{C}_{-1}(\mathbf{e}_{k+1} + \mathbf{e}_{n-k-1}) & 0 \le k \le \lceil \frac{n}{2} \rceil - 2 \\ J\mathcal{C}_{-1}(\mathbf{e}_{n/2}) & k = \lceil \frac{n}{2} \rceil - 1\ (n \text{ even}) \end{cases} \tag{3.21^2}$$

form a basis of γ. *Moreover, the basis* $\{J'_k\}$ *can be expressed in terms of the basis* $\{J_k\}$, $J_k = \gamma_{\mathbf{e}_0+\mathbf{e}_{n-1}}(\mathbf{e}_k)$, *by the following identities:*

$$J'_k = \begin{cases} J_0 + J_{n-1} & k = 0 \\ J_k - J_{k-1} + J_{n-k-1} - J_{n-k} & 1 \le k \le \lceil \frac{n}{2} \rceil - 1, \end{cases} \tag{3.22^1}$$

$$J'_{\lceil \frac{n}{2} \rceil + k} = \begin{cases} J_{k+1} - J_k + J_{n-k-1} - J_{n-k-2} & 0 \leq k \leq \lceil \frac{n}{2} \rceil - 2 \\ J_{n/2} - J_{n/2-1} & k = \lceil \frac{n}{2} \rceil - 1 \ (n \text{ even}). \end{cases} \qquad (3.22^2)$$

Proof. The obvious basis of $\mathcal{C}^S_{-1}$ and $J\mathcal{C}^{SK}_{-1}$ are (3.21^1) and (3.21^2), respectively. Since $\dim \mathcal{C}^S_{-1} + \dim J\mathcal{C}^{SK}_{-1} = n$, the union between ($3.21^1$) and ($3.21^2$) is a basis of γ. In order to prove (3.22), observe that the $\mathbf{e}_0 + \mathbf{e}_{n-1}$-row of the matrices on the right hand-side are equal to the $\mathbf{e}_0 + \mathbf{e}_{n-1}$-row of the matrices J'_k and $J'_{\lceil \frac{n}{2} \rceil + k}$. $\square$

So, $\{J'_0,\ J'_1, \dots,\ J'_{n-1}\}$ is a basis of γ and, therefore,

$$\gamma_A = \sum_{k=0}^{n-1} [B'^{-1}\mathbf{c}']_k J'_k, \quad b'_{ij} = (J'_i, J'_j), \ \ c'_i = (J'_i, A). \qquad (3.23)$$

Notice that $B'^{-1} = \frac{1}{2n}(I + \mathbf{e}_0\mathbf{e}_0^T + \delta_{ne}\mathbf{e}_{n-1}\mathbf{e}_{n-1}^T)$, where $\delta_{ne} = 1$, if n is even, and $\delta_{ne} = 0$, if n is odd. Thus, the complexity of $B'^{-1}\mathbf{c}'$ is determined by the complexity of $\mathbf{c}'$. By the particular form of J'_k, if A is generic, $\mathbf{c}'$ is computable in $O(n^2)$ a.o. and, if $A = T^T T$, in $O(n \log n)$ (see Lemma 5.1 of Appendix).

By (3.22) and by the identities $J_k = \gamma_{\mathbf{e}_0+\mathbf{e}_{n-1}}(\mathbf{e}_k) = Gd(G\mathbf{e}_k)d(\mathbf{w})G$, $w_i = (G(\mathbf{e}_0 + \mathbf{e}_{n-1}))_i^{-1}$, the sum in (3.23) becomes

$$\begin{aligned} \gamma_A \ &= \ [B'^{-1}\mathbf{c}']_0 J'_0 + \textstyle\sum_{k=1}^{\lceil \frac{n}{2} \rceil - 1} [B'^{-1}\mathbf{c}']_k J'_k \\ &\quad + \textstyle\sum_{k=0}^{\lceil \frac{n}{2} \rceil - 2} [B'^{-1}\mathbf{c}']_{\lceil \frac{n}{2} \rceil + k} J'_{\lceil \frac{n}{2} \rceil + k} + \delta_{ne}[B'^{-1}\mathbf{c}']_{n-1} J'_{n-1} \\ &= \ [B'^{-1}\mathbf{c}']_0 Gd(G(\mathbf{e}_0 + \mathbf{e}_{n-1}))d(\mathbf{w})G \\ &\quad + \textstyle\sum_{k=1}^{\lceil \frac{n}{2} \rceil - 1} [B'^{-1}\mathbf{c}']_k Gd(G(\mathbf{e}_k - \mathbf{e}_{k-1} + \mathbf{e}_{n-k-1} - \mathbf{e}_{n-k}))d(\mathbf{w})G \\ &\quad + \textstyle\sum_{k=0}^{\lceil \frac{n}{2} \rceil - 2} [B'^{-1}\mathbf{c}']_{\lceil \frac{n}{2} \rceil + k} Gd(G(\mathbf{e}_{k+1} - \mathbf{e}_k + \mathbf{e}_{n-k-1} - \mathbf{e}_{n-k-2}))d(\mathbf{w})G \\ &\quad + \delta_{ne}[B'^{-1}\mathbf{c}']_{n-1} Gd(G(\mathbf{e}_{n/2} - \mathbf{e}_{n/2-1}))d(\mathbf{w})G. \end{aligned}$$

Thus

$$\gamma_A = Gd(GB^{-1}\mathbf{c})d(G(\mathbf{e}_0 + \mathbf{e}_{n-1}))^{-1}G$$

with

$$\begin{aligned} B^{-1}\mathbf{c} = \gamma_A^T(\mathbf{e}_0 + \mathbf{e}_{n-1}) \ &= \ [B'^{-1}\mathbf{c}']_0(\mathbf{e}_0 + \mathbf{e}_{n-1}) \\ &\quad + \textstyle\sum_{k=1}^{\lceil \frac{n}{2} \rceil - 1} [B'^{-1}\mathbf{c}']_k(\mathbf{e}_k - \mathbf{e}_{k-1} + \mathbf{e}_{n-k-1} - \mathbf{e}_{n-k}) \\ &\quad + \textstyle\sum_{k=0}^{\lceil \frac{n}{2} \rceil - 2} [B'^{-1}\mathbf{c}']_{\lceil \frac{n}{2} \rceil + k}(\mathbf{e}_{k+1} - \mathbf{e}_k + \mathbf{e}_{n-k-1} - \mathbf{e}_{n-k-2}) \\ &\quad + \delta_{ne}[B'^{-1}\mathbf{c}']_{n-1}(\mathbf{e}_{n/2} - \mathbf{e}_{n/2-1}) \end{aligned}$$

i.e. $B^{-1}\mathbf{c}$ is computable from $B'^{-1}\mathbf{c}'$ in $O(n)$ a.o.. This proves, in particular, Theorem 3.5.

Explicit formulas for $(\mathcal{C}_{\pm 1})_A$, η_A, μ_A, $\mathcal{H}_A$, $\mathcal{K}_A$,

The procedures illustrated above to compute $\mathcal{L}_A$ are essentially based on representations of $B^{-1}\mathbf{c}$ in terms of $\mathbf{c}'$ ($\mathcal{L} = \eta$) or in terms of $B'^{-1}\mathbf{c}'$ ($\mathcal{L} = \gamma$), where the J'_k, defining B' and $\mathbf{c}'$, are the sum of a constant number of $I(\mathbf{e}_k)$, $I(\mathbf{e}_k)^T$, $JI(\mathbf{e}_{n-1-k})^T$, $JI(\mathbf{e}_{n-1-k})$ matrices. In the following Theorem 3.7 we give *explicit* formulas for $\mathcal{L}_A$, $\mathcal{L} = \mathcal{C}_1, \mathcal{C}_{-1}, \eta, \mu, \mathcal{H}, \mathcal{K}$. These formulas have been introduced heuristically and then rigorously proved. Notice that only $(\mathcal{C}_{\pm 1})_A$ were previously considered in literature.

Theorem 3.7 *The best l.s. fit to $A \in \mathbb{C}^{n\times n}$ from $\mathcal{L} \in \{\mathcal{C}_{\pm 1}, \mathcal{H}, \mathcal{K}, \eta, \mu\}$ can be represented as*

$$\mathcal{L}_A = U_{\mathcal{L}} d(U_{\mathcal{L}}^T \mathbf{z}) d(U_{\mathcal{L}}^T \mathbf{e}_0)^{-1} U_{\mathcal{L}}^*, \tag{3.24}$$

with $\mathbf{z} = B^{-1}\mathbf{c}$, $J_k = \mathcal{L}(\mathbf{e}_k)$, equal, respectively, to

$$\mathbf{f}_A^{\pm} = \tfrac{1}{n}(\mathbf{r}_A \pm JI(\mathbf{e}_1)\tilde{\mathbf{r}}_A),$$

$$\begin{aligned}&\tfrac{1}{2}(\mathbf{f}_A^{\pm} + \mathbf{f}_{A^T}^{\pm}) + \tfrac{1}{2n}[(I \mp JI(\mathbf{e}_1))\mathbf{h}_A \\ &\qquad -(I(\mathbf{e}_2)^T \mp I(\mathbf{e}_1)J)\tilde{\mathbf{h}}_A - (h_{0,A} \pm \tilde{h}_{n-2,A})\mathbf{e}_0],\end{aligned}$$

$$\begin{aligned}&\tfrac{1}{2}(\mathbf{f}_A^{\pm} + \mathbf{f}_{A^T}^{\pm}) + \tfrac{1}{2n}(I \pm I(\mathbf{e}_1)J)(\mathbf{h}_A + \tilde{\mathbf{h}}_A) \\ &\qquad -\tfrac{1}{n^2}\left[\mathbf{e}\mathbf{e}^T + \mathbf{o}\mathbf{o}^T \pm J(\mathbf{e}\mathbf{o}^T + \mathbf{o}\mathbf{e}^T)\right] I^{\frac{1}{2}}(\mathbf{r}_A + \tilde{\mathbf{r}}_A),\end{aligned}$$

where the upper and the lower signs refer to the cases $\mathcal{C}_1, \mathcal{H}, \eta$ and $\mathcal{C}_{-1}, \mathcal{K}, \mu$, respectively, and $I^{\frac{1}{2}} = \operatorname{diag}(\frac{1}{2}, 1, \ldots, 1)$, $\mathbf{e} = [1\ 0\ 1\ 0 \cdots]^T$, $\mathbf{o} = [0\ 1\ 0\ 1 \cdots]^T$. Moreover, for $\mathcal{L} = \eta, \mu$,

$$\mathcal{L}_A = (\mathcal{C}_{\pm 1})_{\frac{A+A^T}{2}} + J(\mathcal{C}_{\pm 1})_{\frac{JA+AJ}{2}} + JR, \quad R \in \mathcal{C}_{\pm 1}^S$$

where $R = 0$ if $\mathcal{L} = \mu$ and n is even.

Proof. Compute the vector $B^{-1}\mathbf{c}$ for $J_k = \mathcal{L}(\mathbf{e}_k)$. For example, if $\mathcal{L} = \mathcal{C}_{\pm 1}$, then $J_k = P_{\pm 1}^k$. Therefore $[B^{-1}\mathbf{c}]_k = \frac{1}{n}(P_{\pm 1}^k, A) = \frac{1}{n}(r_{k,A} \pm \tilde{r}_{n-k,A})$. The formulas for $\mathcal{L} = \eta, \mu$ are essentially obtained by rewriting in vectorial form some analogous results in [30]. The formulas for $\mathcal{L} = \mathcal{H}, \mathcal{K}$ are new (in [9] only the formula for $\mathcal{H}_T$, T symmetric, is obtained). In order to prove the equality involving $(\mathcal{C}_{\pm 1})_{\frac{JA+AJ}{2}}$, observe that the latter matrix belongs to $\mathcal{C}_{\pm 1}^S$ and use (3.13). $\square$

It is clear, from Theorem 3.7, that the vector $B^{-1}\mathbf{c}$ is computable in $O(n)$ a.o. provided that the inner products in (3.11) are given. Then, the crucial remark in the analysis of the complexity of CGP method with $P = (Ht)_{T^T T}$ (conditions 2 and 3) is that the computation in (3.11) can be performed in at most $O(n \log n)$ a.o.. More precisely, for $A = T^T T$ the formulas in Theorem 3.7 can be simplified by observing that $T^T T$ is symmetric and T is persymmetric ($JT = T^T J$), and therefore, by (3.13), the identities $\tilde{\mathbf{r}}_{T^T T} = \mathbf{r}_{T^T T}$ and $\tilde{\mathbf{h}}_{T^T T} = \mathbf{h}_{T T^T}$ hold. Finally, the fact that T is Toeplitz allows us to apply Lemma 5.1 of Appendix and state the following

Corollary 3.8 *The vector $\mathbf{a} = d(U_{\mathcal{L}}^T \mathbf{e}_0)^{-1} U_{\mathcal{L}}^T B^{-1}\mathbf{c}$ in the equality $\mathcal{L}_{T^T T} = U_{\mathcal{L}} d(\mathbf{a}) U_{\mathcal{L}}^*$, $\mathcal{L} = \mathcal{C}_{\pm 1}, \mathcal{H}, \mathcal{K}, \eta, \mu$, is computable in at most $O(n \log n)$ a.o.. So, the conditions 1, 2, 3 on preconditioners P of $T^T T$ are satisfied for $P = (\mathcal{C}_{\pm 1})_{T^T T}$, $\mathcal{H}_{T^T T}$, $\mathcal{K}_{T^T T}$, $\eta_{T^T T}$, $\mu_{T^T T}$.*

Experimental results

We have applied the $CG(\mathcal{L}_{T^T T})$ method, $\mathcal{L} = I, \eta, \mathcal{H}, \mathcal{C}, \tau, \mathcal{C}_{-1}, \mathcal{K}, \mu, \mathcal{D}$, to the system $T\mathbf{x} = \mathbf{b} = [1\ 1\ \cdots\ 1]^T$ for five different choices of the matrix T. The results are reported in Table 1. If $\mathcal{L}$ is the Jacobi algebra τ, then τ_A can be expressed by (3.24) with $\mathcal{L} = \tau$ and

$$\mathbf{z} = \frac{1}{2n+2}\tau(3\mathbf{e}_0 - \mathbf{e}_2)\Gamma^{-1}\Gamma\mathbf{c}, \ \Gamma\mathbf{c} = \mathbf{r}_A + \tilde{\mathbf{r}}_A - I(\mathbf{e}_2)^T(\mathbf{h}_A + \tilde{\mathbf{h}}_A) \tag{3.25}$$

Table 1: Performance of $\mathcal{L}_{T^TT}$ preconditioners

$\mathcal{L}$	T_I	T_{II}	T_{III}	T_{IV}	T_V
I	148 184	>128 >512	23 22	46 89	69 198
η	24 23	73 283	6 6	10 10	41 78
$\mathcal{H}$	23 22	99 445	6 6	7 9	38 70
$\mathcal{C}$	17 19	94 453	6 6	8 9	33 63
τ	21 23	29 63	5 4	14 16	43 75
$\mathcal{C}_{-1}$	18 19	94 446	6 6	11 14	35 65
$\mathcal{K}$	26 23	93 439	6 6	13 15	41 76
μ	26 25	71 269	6 5	13 16	46 80
$\mathcal{D}$	30 30	>128 >512	9 8	13 14	59 132

where Γ is the same matrix (5.3) of the Appendix. This result follows from the expression of B^{-1}, $J_k = \tau(\mathbf{e}_k)$, found in Example 3 of Section 2. If $\mathcal{L}$ is the dihedral group algebra $\mathcal{D}$, then the first row of $\mathcal{D}_{T^TT}$ can be computed by the formulas

$$\begin{aligned} ([\mathcal{D}_{T^TT}]_{0k})_{k=0}^{\frac{n}{2}-1} &= \tfrac{1}{n}(I + \hat{J}I(\hat{\mathbf{e}}_1))(2\mathbf{r}_{T_1^TT_1} + \mathbf{r}_{T_2^TT_2+T_3^TT_3}), \\ ([\mathcal{D}_{T^TT}]_{0k})_{k=\frac{n}{2}}^{n-1} &= \tfrac{1}{n}[\left(h_{k,T^TT} + h_{\frac{3}{2}n-k-2,TT^T}\right)_{k=\frac{n}{2}}^{n-1} \\ &\quad -I(\hat{\mathbf{e}}_1)\hat{J}\mathbf{h}_{T_1T_1^T+T_3T_3^T} - \mathbf{h}_{T_1^TT_1+T_2^TT_2}] \end{aligned} \tag{3.26}$$

where $\hat{J}$ and $\hat{\mathbf{e}}_1$ are the matrix J and the vector $\mathbf{e}_1 = [0\ 1\ 0 \cdots 0]^T$ of dimension $n/2$ (see Example 5 in Section 2). By T_I, T_{II}, T_{III} we denote the three Toeplitz matrices T considered in [41] in the points (i), (iii), (iv). The elements of the matrices T_{IV} and T_V are defined by

$$\begin{aligned} t_0^{IV} &= t_0^V = 1, \quad t_{-k}^{IV} = \frac{1}{(k+1)^{0.5}}, \quad t_{-k}^V = \frac{1}{|\sin k| + 1}, \\ t_k^{IV} &= t_k^V = \frac{1}{\log(k+1)+1}, \ k \geq 1. \end{aligned}$$

Table 1 shows the number of steps required to satisfy the stopping criterion

$$\frac{\|T^TT\mathbf{x}_k - T^T\mathbf{b}\|}{\|T^T\mathbf{b}\|} < 10^{-7}$$

($\mathbf{x}_0 = \mathbf{0}$) for the two different dimensions $n = 128$ and $n = 512$. Notice that the good performance of τ preconditioners, pointed out in [21] for τ_T, $T = T^T$, seems to hold also for τ_{T^TT}, T non symmetric. But Table 1 also shows that circulant and Hartley type preconditioners may be — in some cases — more efficient.

4 An Efficient $\mathcal{L}^k QN$ Algorithm for the Unconstrained Minimization

In [25] the following $\mathcal{L}QN$ procedure for the minimization of a function $f : \mathbb{R}^n \to \mathbb{R}$ is introduced in terms of a subset $\mathcal{L}$ of $\mathbb{C}^{n\times n}$:

$$\begin{array}{l} \mathbf{x}_0 \in \mathbb{R}^n,\ B_0 = pd\ \ n\times n\ matrix. \\ For\ k=0,1,\dots : \\ \left\{ \begin{array}{l} \mathbf{d}_k = \left\{ \begin{array}{ll} -B_k^{-1}\mathbf{g}_k & \mathcal{S} \\ -\mathcal{L}_{B_k}{}^{-1}\mathbf{g}_k & \mathcal{NS} \end{array} \right. \\ \mathbf{x}_{k+1} = \mathbf{x}_k + \lambda_k \mathbf{d}_k, \quad \lambda_k \in AG_k \\ \mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k,\ \mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k \\ B_{k+1} = \varphi(\mathcal{L}_{B_k}, \mathbf{s}_k, \mathbf{y}_k) \end{array} \right. \end{array} \qquad (\mathcal{L}QN \text{ algorithm})$$

where pd means real symmetric positive definite, $\mathbf{g}_k = \nabla f(\mathbf{x}_k)$, AG_k is the Armijo-Goldstein set

$$\begin{array}{ll} AG_k = \{\ \lambda \in \mathbb{R}^+ : & f(\mathbf{x}_k + \lambda \mathbf{d}_k) \le f(\mathbf{x}_k) + c_1 \lambda \mathbf{d}_k^T \nabla f(\mathbf{x}_k)\ \ \& \\ & \mathbf{d}_k^T \nabla f(\mathbf{x}_k + \lambda \mathbf{d}_k) \ge c_2 \mathbf{d}_k^T \nabla f(\mathbf{x}_k)\ \}, \\ \quad 0 < c_1 < c_2 < 1 & \end{array}$$

[20], and φ is the Hessian approximation updating function

$$\varphi(B, \mathbf{s}, \mathbf{y}) = B + \frac{1}{\mathbf{s}^T \mathbf{y}} \mathbf{y}\mathbf{y}^T - \frac{1}{\mathbf{s}^T B \mathbf{s}} B \mathbf{s}\mathbf{s}^T B. \qquad (4.1)$$

We see that there are two possible definitions of the $\mathcal{L}QN$ search direction $\mathbf{d}_k$, in terms of B_k and in terms of $\mathcal{L}_{B_k}$. The former leads to a Secant method, since B_k solves the secant equation $X\mathbf{s}_{k-1} = \mathbf{y}_{k-1}$. The latter corresponds to a Non Secant one ($\mathcal{L}_{B_k}\mathbf{s}_{k-1} \neq \mathbf{y}_{k-1}$). Notice that if $B_k = \mathcal{L}_{B_k}$ (e.g. when $\mathcal{L} = \mathbb{C}^{n\times n}$), then both $\mathcal{S}$ and $\mathcal{NS}$ $\mathcal{L}QN$ coincide with the $BFGS$ algorithm, the well known quasi-Newton optimization procedure with superlinear rate of convergence [20], [40].

If the set $\mathcal{L}$ satisfies the condition

$$B \text{ pd} \ \Rightarrow\ \mathcal{L}_B \text{ pd}, \qquad (4.2)$$

then the above $\mathcal{L}QN$ algorithm is well defined and yields a strictly decreasing sequence $f(\mathbf{x}_k)$ unless $\mathbf{g}_k = 0$ for some k. In fact, by the structure of φ,

$$B_k \text{ pd} \ \Rightarrow \ \left. \begin{array}{l} \mathcal{L}_{B_k} \text{ pd} \\ \mathbf{s}_k^T \mathbf{y}_k > 0 \end{array} \right\} \Rightarrow\ B_{k+1} \text{ pd} \ \Rightarrow\ \mathcal{L}_{B_{k+1}} \text{ pd}. \qquad (4.3)$$

The condition $\mathbf{s}_k^T \mathbf{y}_k > 0$ is satisfied since $\lambda_k \in AG_k$. The fact that B_{k+1} and $\mathcal{L}_{B_{k+1}}$ are pd guarantees that $\mathbf{d}_{k+1}$ is a descent direction both in the $\mathcal{S}$ and in the $\mathcal{NS}$ case.

Now assume that $\mathcal{L} = sd\ U$ for some unitary matrix U and $\mathcal{L}$ is spanned by real matrices. These assumptions, because of Theorem 2.7(ii), guarantee that (4.2) holds and all vectors $\mathbf{d}_k$ are defined on $\mathbb{R}$. The $\mathcal{L}QN$ algorithm, written in terms of U, becomes

$$\begin{array}{l}
\mathbf{x}_0 \in \mathbb{R}^n, \; B_0 = pd \;\; n \times n \; matrix, \\
U^* \mathbf{d}_0 = \left\{ \begin{array}{ll} -U^* B_0^{-1} \mathbf{g}_0 & \mathcal{S} \\ -d(\mathbf{z}_0)^{-1} U^* \mathbf{g}_0 & \mathcal{NS} \end{array} \right. , \\
\mathbf{d}_0 = U(U^* \mathbf{d}_0). \\
For \; k = 0, 1, \ldots : \\
\left\{ \begin{array}{l}
\mathbf{x}_{k+1} = \mathbf{x}_k + \lambda_k \mathbf{d}_k, \quad \lambda_k \in AG_k \\
\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k, \quad \mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k \\
(4.4^1) \\
\left\{ \begin{array}{ll} (4.4^2) & \mathcal{S} \\ (4.4^3) & \mathcal{NS} \end{array} \right. \\
\mathbf{d}_{k+1} = U(U^* \mathbf{d}_{k+1})
\end{array} \right.
\end{array}$$

where

$$\mathbf{z}_{k+1} = \mathbf{z}_k + \frac{1}{\mathbf{s}_k^T \mathbf{y}_k} |U^* \mathbf{y}_k|^2 - \frac{1}{\mathbf{z}_k^T |U^* \mathbf{s}_k|^2} d(\mathbf{z}_k)^2 |U^* \mathbf{s}_k|^2, \tag{4.4^1}$$

$\mathbf{z}_k$ is the vector $\mathbf{z}_{B_k}$ in the equality $\mathcal{L}_{B_k} = U d(\mathbf{z}_{B_k}) U^*$, and

$$U^* \mathbf{d}_{k+1} = \left\{ \begin{array}{ll}
-d(\mathbf{z}_k^{-1}) U^* \mathbf{g}_{k+1} + \frac{\mathbf{s}_k^T \mathbf{g}_{k+1}}{\mathbf{y}_k^T \mathbf{s}_k} d(\mathbf{z}_k^{-1}) U^* \mathbf{y}_k & \\
\quad + \Big[- \left(1 + \frac{(\mathbf{z}_k^{-1})^T |U^* \mathbf{y}_k|^2}{\mathbf{y}_k^T \mathbf{s}_k} \right) \frac{\mathbf{s}_k^T \mathbf{g}_{k+1}}{\mathbf{y}_k^T \mathbf{s}_k} & \\
\quad + \frac{(\mathbf{z}_k^{-1})^T d(U^T \mathbf{y}_k) U^* \mathbf{g}_{k+1}}{\mathbf{y}_k^T \mathbf{s}_k} \Big] U^* \mathbf{s}_k, & (4.4^2) \\
-d(\mathbf{z}_{k+1})^{-1} U^* \mathbf{g}_{k+1}. & (4.4^3)
\end{array} \right.$$

In (4.4), $|\mathbf{z}|$ ($\mathbf{z}^{-1}$) denotes the vector with elements $|z_i|$ (z_i^{-1}). We have the following results:

1. Each step of $\mathcal{L}QN$ can be implemented by performing two products by U and a constant number of vector inner products.

2. The $\mathcal{NS}$ version of $\mathcal{L}QN$ has a linear rate of convergence.

3. If U defines a fast discrete transform (cost of $U \cdot \mathbf{z} \leq O(n \log n)$), then $\mathcal{L}QN$ can be implemented with $O(n)$ memory allocations and $O(n \log n)$ arithmetic operations per step.

4. If U is the Hartley transform, $U_{ij} = \frac{1}{\sqrt{n}}(\cos \frac{2\pi ij}{n} + \sin \frac{2\pi ij}{n})$, then the $\mathcal{S}$ version of $\mathcal{L}QN$ shows a satisfactory rate of convergence in numerical experiences. The $\mathcal{S}$ $\mathcal{L}QN$ method is, in fact, competitive with the limited memory $BFGS$ method (L-$BFGS$ [40]) in solving large scale minimization problems.

The points (1) and (3) follow immediately from (4.4^1)-(4.4^3). In fact, the two transforms are $U^* \cdot \mathbf{g}_{k+1}$ and $U \cdot (U^* \mathbf{d}_{k+1})$. The point (2) is proved in detail in [25], [28]. Some experiments related to the behaviour of the $\mathcal{S}$ $\mathcal{L}QN$ method cited in (4) are illustrated in [11].

It is essential to notice that the iteration $B_{k+1} = \varphi(\mathcal{L}_{B_k}, \mathbf{s}_k, \mathbf{y}_k)$ is in fact reduced, in the $\mathcal{L}QN$ algorithm, to the updating formula (4.4^1) involving the eigenvalues of $\mathcal{L}_{B_k}$ and $\mathcal{L}_{B_{k+1}}$ only, so that the entire computation runs in terms of single indexed arrays and the space complexity is linear in n. Thus the introduction of $\mathcal{L}QN$ methods has shown that a significant amount of second order information, contained in the eigenvalues $\mathbf{z}_k$ of $\mathcal{L}_{B_k}$, can be sufficient to solve efficiently a minimum unconstrained problem of large dimension. In other words, the information content of $\mathcal{L}_{B_k}$ appears to be sufficiently close to B_k in order to maintain a quasi-newtonian rate of convergence.

In order to improve the $\mathcal{L}QN$ performance, a $\mathcal{L}QN$ algorithm where the space $\mathcal{L}$ is modified at each step has been recently proposed in [27]. More precisely, in [27] it is considered a space $\mathcal{L}^k \subset \mathbb{C}^{n\times n}$ such that the set $\{X \in \mathcal{L}^k : X \text{ is pd and } X\mathbf{s}_{k-1} = \mathbf{y}_{k-1}\}$ is not empty and B_{k+1} is defined by updating a pd matrix of $\mathcal{L}^k$:

$$B_{k+1} = \varphi(A_k, \mathbf{s}_k, \mathbf{y}_k), \quad A_k \in \mathcal{L}^k \text{ and pd.} \tag{4.5}$$

An obvious choice of $\mathcal{L}^k$ is $\mathcal{L}^k = sd\, U_k$, where U_k is a unitary matrix satisfying the inequalities

$$\frac{(U_k^*\mathbf{y}_{k-1})_i}{(U_k^*\mathbf{s}_{k-1})_i} \equiv w_i > 0, \quad i = 1, \ldots, n, \tag{4.6}$$

which is equivalent to say that $\mathcal{L}^k$ satisfies the secant equation $U_k d(\mathbf{w}) U_k^* \mathbf{s}_{k-1} = \mathbf{y}_{k-1}$ and is pd. Numerical experiences with $A_k = U_k d(\mathbf{w}) U_k^*$ in (4.5) (see [27]) show that this criterion (change the space $\mathcal{L}$ at each k and choose U_k in order that (4.6) holds) gives good performances in comparison with the previous $\mathcal{L}QN$ method where $\mathcal{L}$ is fixed. For large scale problems, however, the choice $A_k = U_k d(\mathbf{w}) U_k^*$ does not give good results and the reason is in the fact that the eigenvalues w_i in (4.6) have, in general, no link with the eigenvalues $(U_k^* B_k U_k)_{ii}$ of the best l.s. approximation $\mathcal{L}^k_{B_k}$. So, in the same paper [27] it is suggested to set $A_k = \mathcal{L}^k_{B_k}$ and t ciao $\mathcal{L}^k$ (i.e. U_k) only when the condition (4.6) is not verified (in order to maintain low the complexity per step).

In the following we try to restore a close relation of the updated matrix A_k with the Hessian approximation B_k by using an alternative strategy: choose w_i as the eigenvalues of $\mathcal{L}^{k-1}_{B_k}$, in order to maintain the B_k spectral information, and then choose U_k in order to satisfy the secant equation $U_k d(\mathbf{w}) U_k^* \mathbf{s}_{k-1} = \mathbf{y}_{k-1}$, $\mathbf{w} = (w_i)$. This operation recalls, in spirit, the distinction between *structure* and *information content* of a matrix [7], [48], [8], [5], [6]: in the split $\mathcal{L} = U d(\mathbf{z}) U^*$, U is the same unitary transform for all matrices A of $\mathcal{L}$ (i.e. $U \backsimeq$ structure), whereas $\mathbf{z}$ defines a particular matrix A in the space $\mathcal{L}$ ($\mathbf{z} \backsimeq$ information content). The information content $\mathbf{w}$ regains the correspondent information of B_k, whereas the structure defined by U_k reproduces the fundamental structure of secant methods.

The *Belle Epoque* algorithm

The generic step of the Belle Epoque algorithm is the following:

($\bullet$) Assume that, at a generic step k, a positive definite matrix $A_k = U_k d(\mathbf{w}_k) U_k^*$, U_k unitary, and two vectors $\mathbf{s}_k$, $\mathbf{y}_k$, $\mathbf{s}_k^T \mathbf{y}_k > 0$, are given. The matrix

$$B_{k+1} = \varphi(A_k, \mathbf{s}_k, \mathbf{y}_k) = A_k + \frac{1}{\mathbf{y}_k^T \mathbf{s}_k} \mathbf{y}_k \mathbf{y}_k^T - \frac{1}{\mathbf{s}_k^T A_k \mathbf{s}_k} A_k \mathbf{s}_k \mathbf{s}_k^T A_k \tag{4.7}$$

is positive definite. By projecting the equality (4.7) on $\mathcal{L}^k = sd\, U_k$ and exploiting the linearity of the operator $\mathcal{L}_B$ ($\mathcal{L}_{\alpha B+\beta C} = \alpha\mathcal{L}_B + \beta\mathcal{L}_C$), one obtains the vector $\mathbf{w}_{k+1}$ of the eigenvalues of the positive definite matrix $\mathcal{L}^k_{B_{k+1}}$:

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \frac{1}{\mathbf{s}_k^T\mathbf{y}_k}|U_k^*\mathbf{y}_k|^2 - \frac{1}{\mathbf{w}_k^T|U_k^*\mathbf{s}_k|^2}d(\mathbf{w}_k)^2|U_k^*\mathbf{s}_k|^2 \tag{4.8}$$

where $|\mathbf{z}|$ denotes the vector with elements $|z_i|$. Recall that the eigenvalues $(\mathbf{w}_{k+1})_i$ of $\mathcal{L}^k_{B_{k+1}}$ are related to the eigenvalues $0 < \nu_1^{(k+1)} \leq \ldots \leq \nu_n^{(k+1)}$ of B_{k+1} by the inequalities

$$\begin{array}{rcl} \nu_1^{(k+1)} + \ldots + \nu_r^{(k+1)} & \leq & (\mathbf{w}_{k+1})_{i_1} + \ldots + (\mathbf{w}_{k+1})_{i_r}, \\ (\mathbf{w}_{k+1})_{i_r} + \ldots + (\mathbf{w}_{k+1})_{i_n} & \leq & \nu_r^{(k+1)} + \ldots + \nu_n^{(k+1)}, \end{array} \tag{4.9}$$

where the index-vector $\{i_1, i_2, \ldots, i_n\}$ is a permutation of $\{1, 2, \ldots, n\}$ defined so that $(\mathbf{w}_{k+1})_{i_1} \leq (\mathbf{w}_{k+1})_{i_2} \leq \ldots \leq (\mathbf{w}_{k+1})_{i_n}$ (see [44]). In particular, we have

$$0 < \nu_1^{(k+1)} \leq (\mathbf{w}_{k+1})_{i_1} \leq (\mathbf{w}_{k+1})_s \leq (\mathbf{w}_{k+1})_{i_n} \leq \nu_n^{(k+1)} \tag{4.10}$$

(see also the previous Theorem 2.6(vi)). Now introduce a space $\mathcal{L}^{k+1}$ with an ad hoc structure for the current iteration, i.e. set

$$\mathcal{L}^{k+1} = sd\, U_{k+1}, \quad U_{k+1} \text{ unitary such that } U_{k+1}d(\mathbf{w}_{k+1})U_{k+1}^*\mathbf{s}_k = \mathbf{y}_k. \tag{4.11}$$

Then the positive definite matrix $A_{k+1} := U_{k+1}d(\mathbf{w}_{k+1})U_{k+1}^*$ solves the secant equation as B_{k+1}, and has eigenvalues strictly related to B_{k+1} by (4.9) and (4.10).

Now set

$$\mathbf{d}_{k+1} = \begin{cases} -B_{k+1}^{-1}\nabla f(\mathbf{x}_{k+1}) & \text{(I)} \\ -A_{k+1}^{-1}\nabla f(\mathbf{x}_{k+1}) & \text{(II)} \end{cases}.$$

Since $\mathbf{d}_{k+1}$ is a descent direction (unless $\nabla f(\mathbf{x}_{k+1}) = 0$), the AG_{k+1} set is not empty. Thus, one can set

$$\begin{array}{l} \mathbf{x}_{k+2} = \mathbf{x}_{k+1} + \lambda_{k+1}\mathbf{d}_{k+1}, \quad \lambda_{k+1} \in AG_{k+1}, \\ \mathbf{s}_{k+1} = \mathbf{x}_{k+2} - \mathbf{x}_{k+1}, \\ \mathbf{y}_{k+1} = \nabla f(\mathbf{x}_{k+2}) - \nabla f(\mathbf{x}_{k+1}) \end{array}$$

and observe that $\mathbf{s}_{k+1}^T\mathbf{y}_{k+1} > 0$.

Finally set $k := k+1$ and return to ($\bullet$).

Notice that the Belle Epoque search direction $\mathbf{d}_{k+1}$ can be computed by exploiting the formulas

$$\mathbf{d}_{k+1} = \begin{cases} U_k\Big(- d(\mathbf{w}_k^{-1})U_k^*\mathbf{g}_{k+1} + \frac{\mathbf{s}_k^T\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k}d(\mathbf{w}_k^{-1})U_k^*\mathbf{y}_k\Big) & \\ \quad + \Big[- \Big(1 + \frac{(\mathbf{w}_k^{-1})^T|U_k^*\mathbf{y}_k|^2}{\mathbf{y}_k^T\mathbf{s}_k}\Big)\frac{\mathbf{s}_k^T\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k} & \\ \quad + \frac{(\mathbf{w}_k^{-1})^T d(U_k^T\mathbf{y}_k)U_k^*\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k}\Big]\mathbf{s}_k, & \text{(I)} \\ -U_{k+1}d(\mathbf{w}_{k+1})^{-1}U_{k+1}^*\mathbf{g}_{k+1}. & \text{(II)} \end{cases} \tag{4.12}$$

It follows that the time complexity per step of the Belle Epoque algorithm is determined by the cost of matrix-vector products of type $U_k \cdot \mathbf{z}$ and $U_k^* \cdot \mathbf{z}$, i.e.

$$\text{Time complexity } = O(\, cost(U_k \cdot \mathbf{z})\,) + O(\, cost(U_k^* \cdot \mathbf{z})\,) + O(n).$$

However, the Belle Epoque algorithm does not work in the present form, since the space $\mathcal{L}^{k+1}$ in (4.11) may be not defined. Belle Epoque works if (4.11) is replaced by

$$\mathcal{L}^{k+1} = sd\, U_{k+1}, \quad \begin{array}{l} U_{k+1} \text{ unitary such that} \\ U_{k+1} d(\alpha_{k+1}\tilde{\mathbf{w}}_{k+1}) U_{k+1}^* \mathbf{s}_k = \mathbf{y}_k \\ \text{for suitable } \; \alpha_{k+1} > 0 \; \text{ and} \\ \tilde{\mathbf{w}}_{k+1} = \varepsilon_{k+1}\mathbf{w}_{k+1} + \rho_{k+1}\mathbf{e}, \; (\tilde{\mathbf{w}}_{k+1})_i > 0 \end{array} \tag{4.11$'$}$$

where $\mathbf{e} = [1\ 1\ \cdots\ 1]^T$. In fact, as it is shown after the Remark 0 here below, a unitary matrix U_{k+1} solving (4.11$'$) exists and is obtained as the product of two Householder matrices. So, the time and space complexity of the working Belle Epoque algorithm is $O(n)$ only.

Notice that the matrix $A_{k+1} = U_{k+1} d(\mathbf{w}_{k+1}) U_{k+1}^*$ does not map $\mathbf{s}_k$ into $\mathbf{y}_k$. Thus the Belle Epoque method corresponding to the direction (4.12)-(II), is not secant unless $\mathbf{w}_{k+1}$ is replaced with $\mathbf{z}_{k+1} := \alpha_{k+1}\tilde{\mathbf{w}}_{k+1}$. So, a third Belle Epoque algorithm can be defined, the one corresponding to the search direction

$$\mathbf{d}_{k+1} = -A_{k+1}'^{-1}\mathbf{g}_{k+1}, \quad A'_{k+1} := U_{k+1} d(\mathbf{z}_{k+1}) U_{k+1}^*. \quad \text{(III)} \tag{4.12}$$

Remark 0. By updating $A'_k = U_k d(\mathbf{z}_k) U_k^*$ instead of A_k (i.e. by replacing A_k with A'_k in (4.7), and $\mathbf{w}_k$ with $\mathbf{z}_k$ on the right hand side of (4.8) and of (4.12),(I)), one obtains three alternative versions (I)$'$, (II)$'$, (III)$'$ of Belle Epoque. Notice that in (I), (II), (III) the updated matrix has the same eigenvalues of $\mathcal{L}_{B_k}^{k-1}$, but does not map exactly $\mathbf{s}_{k-1}$ into $\mathbf{y}_{k-1}$. On the contrary, in (I)$'$, (II)$'$, (III)$'$ the updated matrix maps $\mathbf{s}_{k-1}$ into $\mathbf{y}_{k-1}$, but its eigenvalues are a bit different from the eigenvalues of $\mathcal{L}_{B_k}^{k-1}$. $\square$

Consider the following

Problem 4.1 *Given a vector $\mathbf{w}$ with positive entries and two vectors $\mathbf{s}, \mathbf{y}$, $\mathbf{s}^T\mathbf{y} > 0$, find a unitary matrix U, a scalar $\alpha > 0$, and a vector $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$, $\tilde{w}_i > 0$, such that*

$$U d(\alpha\tilde{\mathbf{w}}) U^* \mathbf{s} = \mathbf{y}.$$

Let $H(\mathbf{z})$ denote the Householder matrix corresponding to the vector $\mathbf{z}$, i.e.

$$H(\mathbf{z}) = I - \frac{2}{\|\mathbf{z}\|^2}\mathbf{z}\mathbf{z}^*, \quad \mathbf{z} \in \mathbb{C}^n \tag{4.13}$$

($H(\mathbf{0}) = I$). By using the following lemma (see [27]), one can reformulate Problem 4.1 into a simpler problem.

Lemma 4.2 *Given two vectors $\mathbf{s}, \mathbf{y} \in \mathbb{R}^n \backslash \{\mathbf{0}\}$, let $\mathbf{r},\ \mathbf{x} \in \mathbb{R}^n$ be such that $\|\mathbf{r}\|\|\mathbf{x}\| \neq 0$, and the cosine of the angle between $\mathbf{r}$ and $\mathbf{x}$ is equal to the cosine of the angle between $\mathbf{s}$ and $\mathbf{y}$, i.e.*

$$\frac{\mathbf{r}^T\mathbf{x}}{\|\mathbf{r}\|\|\mathbf{x}\|} = \frac{\mathbf{s}^T\mathbf{y}}{\|\mathbf{s}\|\|\mathbf{y}\|} =: \sqrt{\beta}. \tag{4.14}$$

Set $\mathbf{u} = \mathbf{s} - \mathbf{y} - \left(\frac{\|\mathbf{s}\|}{\|\mathbf{r}\|}\mathbf{r} - \frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\mathbf{x}\right)$, $\mathbf{p} = H(\mathbf{u})\mathbf{s} - \frac{\|\mathbf{s}\|}{\|\mathbf{r}\|}\mathbf{r} = H(\mathbf{u})\mathbf{y} - \frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\mathbf{x}$ *and*

$$U^* = H(\mathbf{p})H(\mathbf{u}). \tag{4.15}$$

Then $U^*\mathbf{s} = \frac{\|\mathbf{s}\|}{\|\mathbf{r}\|}\mathbf{r}$, $U^*\mathbf{y} = \frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\mathbf{x}$.

By Lemma 4.2, Problem 4.1 can be solved by determining $\mathbf{r}, \mathbf{x} \in \mathbb{R}^n$ and $\alpha > 0$, $\tilde{\mathbf{w}}$, $\tilde{w}_i > 0$ such that

$$\frac{\mathbf{r}^T\mathbf{x}}{\|\mathbf{r}\|\|\mathbf{x}\|} = \frac{\mathbf{s}^T\mathbf{y}}{\|\mathbf{s}\|\|\mathbf{y}\|}, \quad d(\alpha\tilde{\mathbf{w}})\frac{\|\mathbf{s}\|}{\|\mathbf{r}\|}\mathbf{r} = \frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\mathbf{x} \tag{4.16}$$

or, equivalently, by solving the following:

Problem 4.3 *Given a vector* $\mathbf{w}$ *with positive entries and two vectors* $\mathbf{s}$, $\mathbf{y}$, $\mathbf{s}^T\mathbf{y} > 0$, *find* $\mathbf{r} \in \mathbb{R}^n$ *and* $\tilde{\mathbf{w}}$ *(i.e.* ε, ρ *in* $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$*) such that*

$$\frac{\mathbf{r}^T d(\tilde{\mathbf{w}})\mathbf{r}}{\|\mathbf{r}\|\|d(\tilde{\mathbf{w}})\mathbf{r}\|} = \frac{\mathbf{s}^T\mathbf{y}}{\|\mathbf{s}\|\|\mathbf{y}\|} =: \sqrt{\beta}. \tag{4.17}$$

The vectors $\mathbf{r}$ *and* $\tilde{\mathbf{w}}$ *obtained in this way,* $\alpha = \frac{\|\mathbf{y}\|}{\|\mathbf{s}\|}\frac{\|\mathbf{r}\|}{\|d(\tilde{\mathbf{w}})\mathbf{r}\|}$, *and* $\mathbf{x} = \gamma d(\tilde{\mathbf{w}})\mathbf{r}$, $\forall\gamma > 0$, *solve* (4.16).

Notice that condition (4.17) can be satisfied only if

$$\sqrt{\beta} \geq \frac{\min_s \tilde{w}_s}{\max_s \tilde{w}_s},$$

thus, a choice of $\tilde{\mathbf{w}}$ different from $\tilde{\mathbf{w}} = \mathbf{w}$ (i.e. a pair (ε, ρ) different from $(1, 0)$) will be necessary to make Problem 4.3 solvable for any $0 < \beta \leq 1$.

If $\mathbf{r}$ has only one nonzero entry, then Problem 4.3 has no solution for $\beta < 1$. Let us try to solve Problem 4.3 with a vector $\mathbf{r}$ of type

$$\mathbf{r} = r_{i_1}\mathbf{e}_{i_1} + r_{i_n}\mathbf{e}_{i_n} \tag{4.18}$$

where $w_{i_1} = \min_s w_s$, $w_{i_n} = \max_s w_s$. The reason for this particular choice of the indeces is linked to the criterion of making (4.17) solvable with $\tilde{\mathbf{w}} = \mathbf{w}$ for most values of β, as it will be clear later. Note that if $n = 2$, then (4.18) represents an arbitrary $\mathbf{r}$.

So, we must determine $r_{i_1}, r_{i_n} \in \mathbb{R}$ and, eventually, $(\varepsilon, \rho) \neq (1, 0)$ such that

$$\frac{\tilde{w}_{i_1}r_{i_1}^2 + \tilde{w}_{i_n}r_{i_n}^2}{\sqrt{r_{i_1}^2 + r_{i_n}^2}\sqrt{\tilde{w}_{i_1}^2 r_{i_1}^2 + \tilde{w}_{i_n}^2 r_{i_n}^2}} = \sqrt{\beta}$$

or, equivalently,

$$(1-\beta)\tilde{w}_{i_1}^2 r_{i_1}^4 - 2r_{i_1}^2 r_{i_n}^2\left(-\tilde{w}_{i_1}\tilde{w}_{i_n} + \beta\frac{\tilde{w}_{i_1}^2 + \tilde{w}_{i_n}^2}{2}\right) + (1-\beta)\tilde{w}_{i_n}^2 r_{i_n}^4 = 0. \tag{4.17$'$}$$

We shall see below how to calculate the scalars r_{i_1}, r_{i_n}, ε, ρ, by considering separately the cases $\beta = 1$ and $0 < \beta < 1$. Once r_{i_1}, r_{i_n}, ε, ρ have been computed, the vectors $\mathbf{r} = r_{i_1}\mathbf{e}_{i_1} + r_{i_n}\mathbf{e}_{i_n}$, $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$, $\mathbf{x} = \gamma(\tilde{w}_{i_1} r_{i_1}\mathbf{e}_{i_1} + \tilde{w}_{i_n} r_{i_n}\mathbf{e}_{i_n})$, $\forall\gamma > 0$, and the scalar

$$\alpha = \frac{\|\mathbf{y}\|}{\|\mathbf{s}\|}\sqrt{\frac{r_{i_1}^2 + r_{i_n}^2}{\tilde{w}_{i_1}^2 r_{i_1}^2 + \tilde{w}_{i_n}^2 r_{i_n}^2}},$$

solve (4.16). As a consequence, the unitary matrix $U = H(\mathbf{u})H(\mathbf{p})$, $\mathbf{p}, \mathbf{u}$ defined in Lemma 4.2, is such that $Ud(\alpha\tilde{\mathbf{w}})U^*\mathbf{s} = \mathbf{y}$, and so the Belle Epoque algorithm modified via (4.11′) works.

Remark 1. By the particular form of $\mathbf{r}$, the above results hold unchanged if the vectors $\alpha\tilde{\mathbf{w}}$ and $\varepsilon\mathbf{w} + \rho\mathbf{e}$, are defined, for $s = i_1, i_n$, by $(\alpha\tilde{\mathbf{w}})_s = \alpha\tilde{w}_s$, $(\varepsilon\mathbf{w} + \rho\mathbf{e})_s = \varepsilon w_s + \rho$, and , for $s \neq i_1, i_n$, by $(\alpha\tilde{\mathbf{w}})_s = \tilde{w}_s$, $(\varepsilon\mathbf{w} + \rho\mathbf{e})_s = w_s$. $\square$

Case $\beta = 1$.
Equation (4.17′) becomes $r_{i_1}^2 r_{i_n}^2 (\tilde{w}_{i_1} - \tilde{w}_{i_n})^2 = 0$. Then set $\tilde{w}_s = w_s$, $s = 1, \dots, n$ or $(\varepsilon, \rho) = (1, 0)$ (we do not need to define $\tilde{\mathbf{w}} \neq \mathbf{w}$, in order to verify (4.17′)), and

$$(r_{i_1}, r_{i_n}) = \begin{cases} (t,h) \neq (0,0) & \tilde{w}_{i_1} = \tilde{w}_{i_n} \\ (t,0) \text{ or } (0,t),\ t \neq 0 & \tilde{w}_{i_1} < \tilde{w}_{i_n} \end{cases}.$$

Case $0 < \beta < 1$.
Divide (4.17′) by $(1-\beta)\tilde{w}_{i_1}^2 r_{i_n}^4$ and find $\frac{r_{i_1}^2}{r_{i_n}^2}$:

$$\frac{r_{i_1}^2}{r_{i_n}^2} = a_\pm = \frac{1}{(1-\beta)\tilde{w}_{i_1}^2}\Bigg[-\tilde{w}_{i_1}\tilde{w}_{i_n} + \beta\left(\frac{(\tilde{w}_{i_1}+\tilde{w}_{i_n})^2}{4} + \frac{(\tilde{w}_{i_1}-\tilde{w}_{i_n})^2}{4}\right) \pm\sqrt{\beta(\tilde{w}_{i_1} - \tilde{w}_{i_n})^2\left[\frac{\beta(\tilde{w}_{i_1}+\tilde{w}_{i_n})^2}{4} - \tilde{w}_{i_1}\tilde{w}_{i_n}\right]}\ \Bigg]. \tag{4.19}$$

Notice that both a_+ and a_- are positive. If $\beta \geq \frac{4w_{i_1}w_{i_n}}{(w_{i_1}+w_{i_n})^2}$ (this condition can be better verified by our particular choice of i_1, i_n), set $\tilde{w}_s = w_s$, $s = 1, \dots, n$ or $(\varepsilon, \rho) = (1, 0)$ (we do not need to define $\tilde{\mathbf{w}} \neq \mathbf{w}$, in order to verify (4.17′)). Otherwise, in order to make $a_\pm$ real, choose $q > 0$ such that $qw_{i_1} \leq \frac{1}{q}w_{i_n}$ and

$$\beta \geq \frac{4qw_{i_1}\frac{1}{q}w_{i_n}}{(qw_{i_1} + \frac{1}{q}w_{i_n})^2},$$

and set $\tilde{w}_{i_1} = qw_{i_1}$, $\tilde{w}_{i_n} = \frac{1}{q}w_{i_n}$,

$$\tilde{w}_s = \begin{cases} w_s & \text{(two)} \\ q\frac{w_{i_1}(w_{i_n}-w_s)}{w_{i_n}-w_{i_1}} + \frac{1}{q}\frac{w_{i_n}(w_s-w_{i_1})}{w_{i_n}-w_{i_1}} & \text{(all)} \end{cases}, \quad s \neq i_1, i_n$$

(see Remark 1) or, equivalently, $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$ where $\varepsilon = \frac{w_{i_n}-q^2w_{i_1}}{q(w_{i_n}-w_{i_1})}$, $\rho = \frac{(q^2-1)w_{i_1}w_{i_n}}{q(w_{i_n}-w_{i_1})}$.

Now $4\tilde{w}_{i_1}\tilde{w}_{i_n}/((\tilde{w}_{i_1} + \tilde{w}_{i_n})^2) \leq \beta < 1$. Thus $(r_{i_1}, r_{i_n}) = (\pm|t|\sqrt{a_+}, t)$ and $(r_{i_1}, r_{i_n}) = (\pm|t|\sqrt{a_-}, t)$ are defined in $\mathbb{R}$ and solve (4.17′) for all $t \neq 0$.

The *Moulin Rouge* algorithm

Observe that if

$$\frac{4\tilde{w}_{i_1}\tilde{w}_{i_n}}{(\tilde{w}_{i_1}+\tilde{w}_{i_n})^2}=\beta, \tag{4.20}$$

then the $a_\pm$ in (4.19) becomes $a_+ = a_- = \tilde{w}_{i_n}/\tilde{w}_{i_1}$. This leads to conceive a more compact and simpler algorithm. Give up the criterion of solving (4.17) with $\tilde{\mathbf{w}} = \mathbf{w}$ (i.e. $(\varepsilon,\rho) = (1,0)$) for all values of β (in the algorithm, for all steps) for which is possible. On the contrary, for each β (in the algorithm, for each step), exploit the parameters ε, ρ in $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$ in order to make the equality (4.20) true.

In detail, let $q > 0$ be such that

$$\frac{4qw_{i_1}\frac{1}{q}w_{i_n}}{(qw_{i_1}+\frac{1}{q}w_{i_n})^2}=\beta.$$

By taking into account the condition $qw_{i_1} \le \frac{1}{q}w_{i_n}$, we obtain $q^2 = \frac{2-\beta-2\sqrt{1-\beta}}{\beta}\frac{w_{i_n}}{w_{i_1}}$, so q is determined:

$$q=\sqrt{\frac{2-\beta-2\sqrt{1-\beta}}{\beta}}\sqrt{\frac{w_{i_n}}{w_{i_1}}}. \tag{4.21}$$

Now set $\tilde{w}_{i_1} = qw_{i_1}$, $\tilde{w}_{i_n} = \frac{1}{q}w_{i_n}$, and

$$\tilde{w}_s = \begin{cases} w_s & \text{(two)} \\ q\frac{w_{i_1}(w_{i_n}-w_s)}{w_{i_n}-w_{i_1}} + \frac{1}{q}\frac{w_{i_n}(w_s-w_{i_1})}{w_{i_n}-w_{i_1}} & \text{(all)} \end{cases}, \quad s \ne i_1, i_n,$$

or, equivalently, $\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}$ where $\varepsilon = \frac{w_{i_n}-q^2w_{i_1}}{q(w_{i_n}-w_{i_1})}$, $\rho = \frac{(q^2-1)w_{i_1}w_{i_n}}{q(w_{i_n}-w_{i_1})}$.

Remark 2. After having computed $\mathbf{w} \equiv \mathbf{w}_{k+1}$ by (4.8), the introduction of the vector $\tilde{\mathbf{w}} = \tilde{\mathbf{w}}_{k+1}$ related to $\mathbf{w}$ by the above identities, corresponds to the definition of a matrix $A'_{k+1} = U_{k+1}d(\alpha\tilde{\mathbf{w}})U^*_{k+1}$ with a condition number greater [smaller] than $\frac{w_{i_n}}{w_{i_1}}$, whenever $\frac{4w_{i_1}w_{i_n}}{(w_{i_1}+w_{i_n})^2} > \; [<] \; \beta$. In fact, the condition number of A'_{k+1} is

$$\mu_2(A'_{k+1}) = \begin{cases} \frac{\max\{w_{i_{n-1}},\tilde{w}_{i_n}\}}{\min\{w_{i_2},\tilde{w}_{i_1}\}} & \text{(two)} \\ \frac{\tilde{w}_{i_n}}{\tilde{w}_{i_1}} & \text{(all)} \end{cases}.$$

□

Then $(r_{i_1}, r_{i_n}) = (\pm|t|\sqrt{\frac{\tilde{w}_{i_n}}{\tilde{w}_{i_1}}}, t)$ satisfy (4.17′) for all $t \ne 0$. Therefore, for such (r_{i_1}, r_{i_n}), the quantities

$$\begin{aligned} &\mathbf{r} = r_{i_1}\mathbf{e}_{i_1} + r_{i_n}\mathbf{e}_{i_n}, \\ &\tilde{\mathbf{w}} = \varepsilon\mathbf{w} + \rho\mathbf{e}, \quad \varepsilon = \tfrac{w_{i_n}-q^2w_{i_1}}{q(w_{i_n}-w_{i_1})}, \;\; \rho = \tfrac{(q^2-1)w_{i_1}w_{i_n}}{q(w_{i_n}-w_{i_1})}, \\ &\alpha = \tfrac{\|\mathbf{y}\|}{\|\mathbf{s}\|}\tfrac{1}{\sqrt{\tilde{w}_{i_1}\tilde{w}_{i_n}}} = \tfrac{\|\mathbf{y}\|}{\|\mathbf{s}\|}\tfrac{1}{\sqrt{w_{i_1}w_{i_n}}}, \\ &\mathbf{x} = \gamma(\tilde{w}_{i_1}r_{i_1}\mathbf{e}_{i_1} + \tilde{w}_{i_n}r_{i_n}\mathbf{e}_{i_n}), \quad \forall\gamma > 0 \end{aligned} \tag{4.22}$$

solve (4.16). As a consequence, we may state the following theorem which gives explicit formulas for the vectors $\mathbf{u}$ and $\mathbf{p}$ in Lemma 4.2:

Theorem 4.4 *Given* $\mathbf{s}, \mathbf{y} \in \mathbb{R}^n$, $\mathbf{s}^T\mathbf{y} > 0$, *and* $\mathbf{w} \in \mathbb{R}^n$, $w_i > 0$, *let* q *and* α, ε, ρ *be defined as in* (4.21) *and* (4.22), *respectively, where* $\sqrt{\beta} = \frac{\mathbf{s}^T\mathbf{y}}{\|\mathbf{s}\|\|\mathbf{y}\|}$. *Moreover, set*

$$\begin{aligned}
\mathbf{u} &= \mathbf{s} - \mathbf{y} + \sigma_{i_1}\mathbf{e}_{i_1} + \sigma_{i_n}\mathbf{e}_{i_n}, \\
\mathbf{p} &= \tfrac{1}{c_1+c_2}\Big[c_1\Big(\mathbf{y} \mp \tfrac{\|\mathbf{y}\|}{\sqrt{1+\mu}}\mathbf{e}_{i_1} - \tfrac{t\|\mathbf{y}\|\sqrt{\mu}}{|t|\sqrt{1+\mu}}\mathbf{e}_{i_n}\Big) \\
&\qquad + c_2\Big(\mathbf{s} \mp \tfrac{\|\mathbf{s}\|\sqrt{\mu}}{\sqrt{1+\mu}}\mathbf{e}_{i_1} - \tfrac{t\|\mathbf{s}\|}{|t|\sqrt{1+\mu}}\mathbf{e}_{i_n}\Big)\Big]
\end{aligned}$$

where

$$\begin{aligned}
&\mu = \tfrac{\tilde{w}_{i_n}}{\tilde{w}_{i_1}} = \tfrac{w_{i_n}}{q^2 w_{i_1}}, \\
&\sigma_{i_1} = -\tfrac{1}{\sqrt{1+\mu}}(\pm\|\mathbf{s}\|\sqrt{\mu} \mp \|\mathbf{y}\|), \\
&\sigma_{i_n} = -\tfrac{t}{|t|\sqrt{1+\mu}}(\|\mathbf{s}\| - \|\mathbf{y}\|\sqrt{\mu}), \\
&c_1 = (\mathbf{s}-\mathbf{y})^T\mathbf{s} + \sigma_{i_1}s_{i_1} + \sigma_{i_n}s_{i_n}, \\
&c_2 = -(\mathbf{s}-\mathbf{y})^T\mathbf{y} - \sigma_{i_1}y_{i_1} - \sigma_{i_n}y_{i_n}.
\end{aligned}$$

Then

$$H(\mathbf{u})H(\mathbf{p})d(\alpha(\varepsilon\mathbf{w} + \rho\mathbf{e}))H(\mathbf{p})H(\mathbf{u})\mathbf{s} = \mathbf{y}. \tag{4.23}$$

Proof. Use Lemma 4.2 and the equalities

$$\begin{aligned}
&\|\mathbf{r}\|^2 = t^2(1+\mu), \quad \|\mathbf{x}\|^2 = \gamma^2\tilde{w}_{i_1}\tilde{w}_{i_n}\|\mathbf{r}\|^2, \\
&2\sqrt{\mu} = \tfrac{\mathbf{s}^T\mathbf{y}}{\|\mathbf{s}\|\|\mathbf{y}\|}(1+\mu), \quad \sigma_{i_1}^2 + \sigma_{i_n}^2 = \|\mathbf{s}-\mathbf{y}\|^2.
\end{aligned}$$

Observe that in the (two) case the expression $\alpha(\varepsilon\mathbf{w} + \rho\mathbf{e})$ is defined, for $s = i_1, i_n$, by $[\alpha(\varepsilon\mathbf{w} + \rho\mathbf{e})]_s = \alpha(\varepsilon w_s + \rho)$, and, for $s \neq i_1, i_n$, by $[\alpha(\varepsilon\mathbf{w} + \rho\mathbf{e})]_s = w_s$. □

Notice that, by Theorem 2.7(iii), the eigenvalues of A'_{k+1} in the Moulin Rouge algorithm, case (all), are

$$\begin{aligned}
\alpha(\tilde{w}_{k+1})_s &= \alpha(\varepsilon(w_{k+1})_s + \rho) \\
&= \alpha(\varepsilon[U_k^* B_{k+1} U_k]_{ss} + \rho) \\
&= [U_k^*(\alpha(\varepsilon B_{k+1} + \rho I))U_k]_{ss}
\end{aligned}$$

i.e. they are the eigenvalues of the matrix $\mathcal{L}^k_{\alpha\varepsilon B_{k+1}+\alpha\rho I} = \alpha\mathcal{L}^k_{\varepsilon B_{k+1}+\rho I} = \alpha\varepsilon\mathcal{L}^k_{B_{k+1}} + \alpha\rho I$ where

$$\alpha = \frac{\|\mathbf{y}\|}{\|\mathbf{s}\|}\frac{1}{\sqrt{w_{i_1}w_{i_n}}}, \quad \varepsilon = \frac{w_{i_n} - q^2 w_{i_1}}{q(w_{i_n} - w_{i_1})}, \quad \rho = \frac{(q^2-1)w_{i_1}w_{i_n}}{q(w_{i_n} - w_{i_1})}.$$

Problem 6: Can Moulin Rouge be generalized to $\mathbf{r} = \sum_{k=1}^n r_k\mathbf{e}_k$? I.e., is it possible to introduce a vector $\tilde{\mathbf{w}}$ (satisfying an equality of type (4.20)) for which (4.17) has a simple solution vector $(r_1, \ldots, r_n)$?

Finally, we resume here below the basic instructions for each step of Belle Epoque and

Moulin Rouge algorithms:

$$
\begin{array}{l}
\mathbf{x}_0 \in \mathbb{R}^n,\ U_0 =\ n\times n \text{ unitary matrix, } \mathbf{w}_0 = [1\,1\cdots 1]^T,\ \mathbf{z}_0 = \mathbf{w}_0,\\
U_0^*\mathbf{d}_0 = -U_0^*\mathbf{g}_0,\ \mathbf{d}_0 = U_0(U_0^*\mathbf{d}_0).\\
For\ k = 0,1,\dots :\\
\left\{
\begin{array}{l}
\mathbf{x}_{k+1} = \mathbf{x}_k + \lambda_k\mathbf{d}_k, \quad \lambda_k \in AG_k\\
\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k, \quad \mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k,\\
(4.8),\\
\text{Calculate } \alpha_{k+1}, \varepsilon_{k+1}, \rho_{k+1}, \mathbf{u}_{k+1}, \mathbf{p}_{k+1} \text{ such that}\\
H(\mathbf{u}_{k+1})H(\mathbf{p}_{k+1})d(\alpha_{k+1}(\varepsilon_{k+1}\mathbf{w}_{k+1} + \rho_{k+1}\mathbf{e}))H(\mathbf{p}_{k+1})H(\mathbf{u}_{k+1})\mathbf{s}_k = \mathbf{y}_k,\\
\mathbf{z}_{k+1} = \alpha_{k+1}(\varepsilon_{k+1}\mathbf{w}_{k+1} + \rho_{k+1}\mathbf{e}),\\
U_{k+1} = H(\mathbf{u}_{k+1})H(\mathbf{p}_{k+1}),\\
\mathbf{d}_{k+1} = \left\{
\begin{array}{ll}
U_k(U_k^*\mathbf{d}_{k+1}),\ (4.24^1) & \text{(I)}\\
U_{k+1}(U_{k+1}^*\mathbf{d}_{k+1}),\ (4.24^2) & \text{(II)}\\
U_{k+1}(U_{k+1}^*\mathbf{d}_{k+1}),\ (4.24^3) & \text{(III)}
\end{array}\right.
\end{array}\right.
\end{array}
$$

where

$$
\begin{array}{rcll}
U_k^*\mathbf{d}_{k+1} & = & -d(\mathbf{w}_k^{-1})U_k^*\mathbf{g}_{k+1} + \frac{\mathbf{s}_k^T\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k}d(\mathbf{w}_k^{-1})U_k^*\mathbf{y}_k & \\
 & & +\Big[-\left(1 + \frac{(\mathbf{w}_k^{-1})^T|U_k^*\mathbf{y}_k|^2}{\mathbf{y}_k^T\mathbf{s}_k}\right)\frac{\mathbf{s}_k^T\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k} & \\
 & & +\frac{(\mathbf{w}_k^{-1})^T d(U_k^T\mathbf{y}_k)U_k^*\mathbf{g}_{k+1}}{\mathbf{y}_k^T\mathbf{s}_k}\Big]U_k^*\mathbf{s}_k, & (4.24^1)\\
U_{k+1}^*\mathbf{d}_{k+1} & = & -d(\mathbf{w}_{k+1})^{-1}U_{k+1}^*\mathbf{g}_{k+1}, & (4.24^2)\\
U_{k+1}^*\mathbf{d}_{k+1} & = & -d(\mathbf{z}_{k+1})^{-1}U_{k+1}^*\mathbf{g}_{k+1}. & (4.24^3)
\end{array}
$$

Remark 3. Following Remark 0, three alternative Belle Epoque (Moulin Rouge) algorithms (I)′, (II)′, (III)′ can be obtained by replacing in the above scheme, on the right hand side of (4.8) and of (4.24^1), the vector $\mathbf{w}_k$ with $\mathbf{z}_k$. □

5 Appendix

Lemma 5.1 *For $A = T^TT$ with $T = (t_{i-j})_{i,j=0}^{n-1}$, $t_k \in \mathbb{C}$, the inner products in* (3.11) *can be computed in at most $O(n\log n)$ a.o. via the formulas $\tilde{\mathbf{r}}_{T^TT} = \mathbf{r}_{T^TT}$, $\tilde{\mathbf{h}}_{T^TT} = \mathbf{h}_{TT^T}$,*

$$\mathbf{r}_{T^TT} = \left[DI(T^T\mathbf{e}_0)^T + I(T\mathbf{e}_0 - t_0\mathbf{e}_0)D\right]T\mathbf{e}_0 + I(T^T\mathbf{e}_0 - t_0\mathbf{e}_0)DT^T\mathbf{e}_0, \tag{5.1}$$

$$\mathbf{h}_{T^TT} = \Gamma^{-1}\mathbf{y}, \quad \mathbf{y} = \begin{array}{l} I(T^T\mathbf{e}_0 - t_0\mathbf{e}_0)^T(T^T\mathbf{e}_0 - t_0\mathbf{e}_0) + 2I(T^T\mathbf{e}_0)^TT\mathbf{e}_0 + \\ \left[2I(JT\mathbf{e}_0)J - JI(JI(\mathbf{e}_2)T\mathbf{e}_0)\right](T\mathbf{e}_0 - t_0\mathbf{e}_0), \end{array} \tag{5.2}$$

where $D = \mathrm{diag}(n-j,\ j = 0,\dots,n-1)$, $I(\mathbf{z})$ is the upper triangular Toeplitz matrix defined in (3.12)*, and*

$$\Gamma = \begin{bmatrix} 2 & & & & & \\ 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & -1 & \ddots & \ddots & & \\ & & \ddots & \ddots & 1 & \\ & & & -1 & 0 & 1 \end{bmatrix}. \tag{5.3}$$

Proof. Rewrite T as $T = T_l + T_u + t_0 I$ where T_u (T_l) is the strictly upper (lower) triangular part of T. Then $T^T T = T_u^T T_u + T_l^T T_l + W$ where W is a symmetric Toeplitz matrix whose first column is $\mathbf{w} = W\mathbf{e}_0 = I(T^T\mathbf{e}_0)^T T\mathbf{e}_0 = I(T\mathbf{e}_0)^T T^T\mathbf{e}_0$. Formula (5.1) follows, by linearity, from the identities

$$\mathbf{r}_W = D\mathbf{w}, \quad \mathbf{r}_{T_u^T T_u} = T_u D T_u^T \mathbf{e}_0, \quad \mathbf{r}_{T_l^T T_l} = \tilde{\mathbf{r}}_{T_l T_l^T} = \mathbf{r}_{T_l T_l^T} = T_l^T D T_l \mathbf{e}_0,$$

and $\mathbf{r}_{T^T T} = \mathbf{r}_{T_u^T T_u} + \mathbf{r}_{T_l^T T_l} + \mathbf{r}_W$. Regarding formula (5.2) obviously we have

$$h_{0,W} = w_0, \quad h_{1,W} = 2w_1, \quad h_{k,W} = h_{k-2,W} + 2w_k, \; 2 \le k \le n-1.$$

Now let R_u (R_l) be the lower triangular $(2n+1)\times n$ Toeplitz matrix with first column $[0\; t_{-1} \cdots t_{-n+1}\; 0\; -2t_{-n+1} \cdots -2t_{-1}\; 0]^T \quad ([0\; t_1 \cdots t_{n-1}\; 0\; -2t_{n-1} \cdots -2t_1\; 0]^T)$ and let q_i^u (q_i^l), $i = 0, 1, \ldots, 2n$, be the entries of the vector $R_u T_u^T \mathbf{e}_0$ ($R_l T_l \mathbf{e}_0$). Then the identity

$$[T_u^T T_u]_{ij} = \begin{cases} t_{-i}t_{-j} + [T_u^T T_u]_{i-1,j-1} & 1 \le i, j \le n-1 \\ 0 & \text{otherwise} \end{cases}$$

yields the equations

$$\begin{array}{l} h_{0,T_u^T T_u} = q_0^u = 0, \quad h_{1,T_u^T T_u} = q_1^u = 0, \\ h_{k,T_u^T T_u} - h_{k-2,T_u^T T_u} = q_k^u, \quad 2 \le k \le 2n-2, \\ h_{2n-3,T_u^T T_u} = -q_{2n-1}^u, \quad h_{2n-2,T_u^T T_u} = -q_{2n}^u/2 \end{array} \tag{5.4}$$

where $h_{2n-i-2,T_u^T T_u} \equiv \tilde{h}_{i,T_u^T T_u}$, $0 \le i \le 2n-2$. As a consequence, one also obtains

$$h_{0,T_l^T T_l} = -q_{2n}^l/2, \; h_{1,T_l^T T_l} = -q_{2n-1}^l, \; h_{k,T_l^T T_l} = h_{k-2,T_l^T T_l} - q_{2n-k}^l, \; 2 \le k \le n-1.$$

Finally, by linearity,

$$h_{0,T^T T} = y_0/2, \quad h_{1,T^T T} = y_1, \quad h_{k,T^T T} = h_{k-2,T^T T} + y_k, \; 2 \le k \le n-1$$

where $y_k = q_k^u - q_{2n-k}^l + 2w_k$, $0 \le k \le n-1$, i.e. the desired formula (5.2) holds. □

Notice that Lemma 5.1 essentially reports in a compact form some Lemmas of Potts-Steidl [41]. However, the formula (5.1) for $\mathbf{r}_{T^T T}$ is simpler than the analogs in [41] as it is obtained by a different splitting of the Toeplitz matrix T. Moreover the *boundary* value difference equations (5.4) are not pointed out in [41].

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