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Matrix algebras in optimal preconditioning[☆]

Carmine Di Fiore, Paolo Zellini*

*Dipartimento di Matematica, Università di Roma “Tor Vergata”, Via della Ricerca Scientifica,
00133 Rome, Italy*

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Abstract

The theory and the practice of optimal preconditioning in solving a linear system by iterative processes is founded on some theoretical facts understandable in terms of a class \mathbb{V} of spaces of matrices including diagonal algebras and group matrix algebras. The \mathbb{V} -structure lets us extend some known crucial results of preconditioning theory and obtain some useful information on the computability and on the efficiency of *new* preconditioners. Three preconditioners not yet considered in literature, belonging to three corresponding algebras of \mathbb{V} , are analyzed in detail. Some experimental results are included. © 2001 Elsevier Science Inc. All rights reserved.

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1. Introduction

This paper is chiefly devoted to the study of preconditioners in solving a linear system $Ax = b$ by the conjugate gradient (CG) method, taking especially into account the case where the $n \times n$ matrix A has Toeplitz form. In fact Strang [35], Strang and Edelman [36] and Chan [18] were the first to show how the use of preconditioners makes the CG a suitable method to solve linear Toeplitz systems.

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* Corresponding author. Fax: +39-6-72594699.

E-mail address: zellini@mat.uniroma2.it (P. Zellini).

It is well known that a good preconditioner is a matrix S which approximates A and can be inverted by efficient algorithms, usually based on fast transforms (FFT, sine or cosine transforms, Hartley transform). The preconditioner approximating A is then regularly chosen in a space of matrices which can be put simultaneously in diagonal form through unitary matrices defining the above efficient transforms.

Among the algebras of matrices simultaneously diagonalized by unitary transforms considered in preconditioning literature we have the following:

1. $C = \{\text{circulant matrices}\}$;
2. $C_\beta = \{\beta\text{-circulant with } |\beta| = 1\}$;
3. $\tau = \{\text{matrices diagonalized by the sine transform}\}$;
4. $\mathcal{H} = \{\text{matrices diagonalized by the Hartley transform}\}$;
5. Hessenberg (or Jacobi) algebras = $\{\text{matrices diagonalized by trigonometric transforms}\}$.

The “good” preconditioners S of a positive definite matrix A , chosen among the previous “diagonal” spaces or algebras (algebras of matrices simultaneously diagonalizable) also satisfy the further conditions:

- The spectrum of S is “contained” in the spectrum of A , i.e., $\min \lambda(S) \geq \min \lambda(A)$ and $\max \lambda(S) \leq \max \lambda(A)$.
- Computing S and solving $Sz = f$ has complexity at most $k\Phi(n)$, where $\Phi(n)$ is the amount of operations to calculate the matrix–vector product Af and k is constant.
- The eigenvalues of $S^{-1}A$ are clustered around 1.

It is clearly important to make the preconditioned algorithm substantially faster than the unpreconditioned, and to this aim the application of the preconditioner (computing S and solving $Sz = f$) should be faster than the multiplication Af (i.e., $k < 1$). Typically one tries to solve $Sz = f$ by two *fast* n -transforms, whereas, when A is Toeplitz, two fast $2n$ -transforms (FFT or, for $a_{ij} = a_{ji}$, Hartley transform) are required to compute Af .

One aim of this paper is to approach, from a more general point of view, some theoretical facts that justify the theory and the practice of optimal preconditioning, so that good preconditioners may be chosen, in principle, in a class of algebras of matrices including, *as a proper subset*, the spaces of matrices simultaneously diagonalized by unitary transforms (SDU).

This class of algebras is defined by a specific property (*) and includes, as significative instances, all spaces SDU and all group algebras (GAs). The property (*) is better understandable if it is related to a class \mathbb{V} of n -dimensional spaces of matrices (defined in Section 2) generalizing the notions of Hessenberg algebra (HA) [10,23,24] and of h -space [3,4,21] exploited in solving “structured” linear systems by the displacement rank technique (although the concept of \mathbb{V} -structure has its last root in a previous task of looking for the explicit form of closed and/or commutative n -dimensional spaces spanned by $(0, 1)$ matrices [4,5,26,43]).

The most interesting result concerning a space \mathcal{L} of class \mathbb{V} satisfying $(*)$ is explained in Theorem 2.11 of Section 2: if \mathcal{L}_A is the best fit to a positive definite matrix A from \mathcal{L} (in the Frobenius norm $\|\cdot\|_F$), then \mathcal{L}_A is positive definite; moreover, $\min \lambda(\mathcal{L}_A) \geq \min \lambda(A)$ and $\max \lambda(\mathcal{L}_A) \leq \max \lambda(A)$. This theorem extends some previous results holding for $\mathcal{L} =$ diagonal algebra UDU^H , where U is a fixed unitary matrix [14,28,33,38].

In Sections 3–6, is studied the more concrete possibility of exploiting some special algebras of class \mathbb{V} in preconditioning technique. We consider a class of symmetric 1-spaces which contains, besides the Hartley algebra \mathcal{H} [8], four other algebras of matrices simultaneously diagonalizable by Hartley-type transforms. These algebras—denoted, respectively, by the symbols η , μ , \mathcal{K} , γ —have not yet been considered in preconditioning literature (only three of them have been recently used in displacement-rank decompositions of Toeplitz-like matrices in [21]). Notice that γ is not always, i.e., for all n , a 1-space, but it is, in any case, a space of class \mathbb{V} .

The most promising preliminary result regards the algebras η and μ : η_A and μ_A , the best fits to A (symmetric and persymmetric) from η and μ , are approximations to A better than the corresponding best fits, respectively, from C , \mathcal{H} and C_{-1} , \mathcal{K} (see Theorem 3.6). This result applies, in particular, to $A = T$, where T is a symmetric Toeplitz matrix.

In Section 4, \mathcal{L}_A , for $\mathcal{L} \in \{\eta, \mu\}$, is effectively computed. Some formulas are first indicated for a generic A , then the case where $A = T$ is analyzed in detail.

In Section 5 (Theorem 5.1), it is proved that the algebras η , μ , \mathcal{K} are competitive candidates for preconditioning in iterative processes: if $A = T$, where T is a symmetric Toeplitz matrix belonging to the Wiener class, with positive generating function, and \mathcal{L}_T is the best fit to T from $\mathcal{L} \in \{\eta, \mu, \mathcal{K}\}$, then the eigenvalues of $\mathcal{L}_T^{-1}T$ are clustered around 1. In Section 6 (Theorem 6.1), the explicit formulas of $\|\mathcal{L}_T - T\|_F^2$ are written for $\mathcal{L} = \eta, \mathcal{H}, C, \tau, C_{-1}, \mathcal{K}, \mu$. These formulas are useful for a sharper comparison between different optimal preconditioners, and some of them give further information regarding the problem risen in Theorem 3.6.

Obviously, the efficiency of the new preconditioners $\eta_A, \mu_A, \mathcal{K}_A$ depends upon the complexity of the transforms $Q_\eta, Q_\mu, Q_{\mathcal{K}}$ diagonalizing, respectively, η, μ, \mathcal{K} . $Q_{\mathcal{K}}$ has the same complexity of the Hartley transform [21]; Q_η is reduced to $Q_{\mathcal{K}}$ via formula (3.16) and Q_μ can be defined in terms of the new fast transform $G = Q_\gamma$ diagonalizing γ (see (3.18) and (3.20)). It would be useful to develop fast algorithms to calculate η and μ transforms directly, i.e., without reference to other transforms.

Some experimental data confirm the theoretical results.

2. Best least-squares fit to a matrix from spaces of class \mathbb{V}

Given a square matrix A of dimension n and a space of matrices \mathcal{L} we are interested to elements of \mathcal{L} which best approximate A in some given norm. We show that if the norm is the Frobenius norm, then there is only one element in \mathcal{L} , \mathcal{L}_A , with such

property. An *explicit* formula for \mathcal{L}_A is found in Theorem 2.2 (in terms of a basis of \mathcal{L} and a_{ij}). Under suitable conditions on \mathcal{L} , it is shown that \mathcal{L}_A inherits some properties from A (\mathcal{L}_A is Hermitian if $A = A^H$ and \mathcal{L}_A is positive definite if A is positive definite), and that the coefficient matrix of the linear system whose solution defines \mathcal{L}_A (see Theorem 2.2) is an element of \mathcal{L} . In particular, in Theorem 2.11, we state that if A is Hermitian and \mathcal{L} satisfies a special condition $(*)$ holding for both GAs and spaces of matrices simultaneously diagonalized by a unitary transform, then the greatest (smallest) eigenvalue of \mathcal{L}_A is smaller (greater) than the greatest (smallest) eigenvalue of A . These results, which were previously known under less general conditions, will be exploited in Sections 4 and 5 in order to calculate \mathcal{L}_A for some special spaces \mathcal{L} (studied in Section 3), and then to study \mathcal{L}_A as a preconditioner of positive definite linear systems $Ax = b$. The most significant results of this section are obtained assuming that \mathcal{L} is a space of *class* \mathbb{V} satisfying the condition $(*)$. The notion of class \mathbb{V} is a significant generalization of the previous notions of HA [10,23,24] and of h -space [3,4,21]. An important feature of \mathbb{V} , with respect to HAs and h -spaces, is that it includes any space of simultaneously diagonalizable matrices. In fact, any space consisting in all the polynomials in a nonderogatory matrix is an element of \mathbb{V} (Theorem 2.5).

Let $M_n(\mathbb{C})$ be the set of all $n \times n$ matrices with complex entries. Let \mathcal{L} be a (linear) subspace of $M_n(\mathbb{C})$ of dimension m . Let $A \in M_n(\mathbb{C})$ be fixed, and consider the minimum problem

$$\min_{X \in \mathcal{L}} \|X - A\|, \quad (2.1)$$

where $\|\cdot\|$ is a matrix norm on $M_n(\mathbb{C})$.

Proposition 2.1. *Problem (2.1) has always at least one solution.*

Proof. Let $J_k, k = 1, \dots, m$, be m matrices spanning \mathcal{L} . Then

$$\left\| \sum_{k=1}^m z_k J_k - A \right\| \geq \left\| \sum_{k=1}^m z_k J_k \right\| - \|A\| \geq \|z\|_2 b - \|A\|, \quad \forall z \in \mathbb{C}^m, \quad (2.2)$$

for a constant $b > 0$. Set $c = \inf\{\|\sum_{k=1}^m z_k J_k - A\| : z_k \in \mathbb{C}\}$. By (2.2) we have

$$\begin{aligned} c &= \inf \left\{ \left\| \sum_{k=1}^m z_k J_k - A \right\| : \|z\|_2 \leq \frac{c + 1 + \|A\|}{b} \right\} \\ &= \min \left\{ \left\| \sum_{k=1}^m z_k J_k - A \right\| : \|z\|_2 \leq \frac{c + 1 + \|A\|}{b} \right\}. \quad \square \end{aligned}$$

As it is stated in the following theorem (Theorem 2.2), if the norm in (2.1) is the Frobenius norm $\|X\|_F = (\sum_{i,j=1}^n |x_{ij}|^2)^{1/2}$ (as it will be throughout the paper), then problem (2.1) has a unique solution. This result follows from the well-known

projection theorem [11,32] for Hilbert spaces. In fact $M_n(\mathbb{C})$ is a Hilbert space with the inner product

$$(A, A') = \sum_{r,t=1}^n \bar{a}_{rt} a'_{rt}, \quad A, A' \in M_n(\mathbb{C}), \quad (2.3)$$

the norm induced by (2.3) is just the Frobenius norm and \mathcal{L} is a closed (with respect to $\|\cdot\|_F$) subspace of $M_n(\mathbb{C})$.

Theorem 2.2. *If the norm in (2.1) is the Frobenius norm, then there exists a unique matrix \mathcal{L}_A of \mathcal{L} solving problem (2.1). The matrix \mathcal{L}_A , which is referred to as the best least-squares (l.s.) fit to A from \mathcal{L} , is equivalently defined by the condition*

$$(A - \mathcal{L}_A, X) = 0 \quad \forall X \in \mathcal{L}, \quad (2.4)$$

i.e., \mathcal{L}_A is the unique element of \mathcal{L} such that $A - \mathcal{L}_A$ is orthogonal to \mathcal{L} .

If \mathcal{L} is spanned by the matrices J_k , $k = 1, \dots, m$, then $\mathcal{L}_A = \sum_{k=1}^m [B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}]_k J_k$, where $B_{\mathcal{L}}$ is the $m \times m$ Hermitian positive definite matrix

$$[B_{\mathcal{L}}]_{ij} = \sum_{r,t=1}^n \overline{[J_i]_{rt}} [J_j]_{rt} = (J_i, J_j), \quad i, j = 1, \dots, m, \quad (2.5)$$

and $\mathbf{c}_{\mathcal{L},A}$ is the $m \times 1$ vector

$$[\mathbf{c}_{\mathcal{L},A}]_i = \sum_{r,t=1}^n \overline{[J_i]_{rt}} a_{rt} = (J_i, A), \quad i = 1, \dots, m \quad (2.6)$$

(notice that $B_{\mathcal{L}}$ and $\mathbf{c}_{\mathcal{L},A}$ depend upon the choice of the J_k 's).

Remark 1. A direct proof of Theorem 2.2 is obtained by using the identity

$$\left\| \sum_{k=1}^m z_k J_k - A \right\|_F^2 = \mathbf{z}^H B_{\mathcal{L}} \mathbf{z} - 2 \operatorname{Re}(\mathbf{z}^H \mathbf{c}_{\mathcal{L},A}) + \|A\|_F^2, \quad \mathbf{z} \in \mathbb{C}^m. \quad (2.7)$$

Identity (2.7) with $A = 0$ and the linear independence of the J_k imply that $\mathbf{z}^H B_{\mathcal{L}} \mathbf{z} = \|\sum_{k=1}^m z_k J_k\|_F^2 > 0 \quad \forall \mathbf{z} \in \mathbb{C}^m, \mathbf{z} \neq 0$. Thus, $B_{\mathcal{L}}$ is positive definite and the matrix $\mathcal{L}_A \equiv \sum_{k=1}^m [B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}]_k J_k$ is well defined. Moreover, by (2.7) we have, for an “increment” $\sum_{k=1}^m z_k J_k$,

$$\begin{aligned} \left\| \mathcal{L}_A + \sum_{k=1}^m z_k J_k - A \right\|_F^2 &= \|\mathcal{L}_A - A\|_F^2 + \mathbf{z}^H B_{\mathcal{L}} \mathbf{z} \\ &> \|\mathcal{L}_A - A\|_F^2 \quad \forall \mathbf{z} \in \mathbb{C}^m, \mathbf{z} \neq 0. \end{aligned}$$

Remark 2. If A is real and there exist real matrices J_k spanning \mathcal{L} , then also \mathcal{L}_A is real. In fact $\operatorname{Re}(\mathcal{L}_A) \in \mathcal{L}$ and $\|\mathcal{L}_A - A\|_F^2 = \|\operatorname{Re}(\mathcal{L}_A) - A\|_F^2 + \|\operatorname{Im}(\mathcal{L}_A)\|_F^2$;

thus, $\text{Im}(\mathcal{L}_A) \neq 0$ would imply that $\text{Re}(\mathcal{L}_A)$ approximates A better than \mathcal{L}_A , which is absurd. If A is real, but not all the J_k 's are real, then \mathcal{L}_A may be not real, as in the following example:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad a_{ij} \in \mathbb{R},$$

$$\mathcal{L} = \left\{ \begin{pmatrix} z_1 & z_2 \\ i z_2 & z_1 \end{pmatrix} : z_k \in \mathbb{C} \right\}$$

$$\Rightarrow \mathcal{L}_A = \frac{1}{2} \begin{pmatrix} a_{11} + a_{22} & a_{12} - i a_{21} \\ a_{21} + i a_{12} & a_{11} + a_{22} \end{pmatrix}.$$

If $\|\cdot\|$ is a matrix norm different from the Frobenius norm, minimum problem (2.1) can have more than one solution. For example, in case $\|\cdot\|$ is the matrix 1-norm, $\|X\| = \max_j \sum_{i=1}^n |x_{ij}|$,

$$A = \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathcal{L} = \left\{ \begin{pmatrix} z_1 & z_2 & z_3 \\ z_3 & z_1 & z_2 \\ z_2 & z_3 & z_1 \end{pmatrix} : z_i \in \mathbb{C} \right\}, \quad (2.8)$$

we have $\|X - A\| \geq \frac{1}{2} \forall X \in \mathcal{L}$, and therefore besides the Strang preconditioner of A (which is the identity matrix, see [12,35,36]) any other Hermitian matrix of \mathcal{L} , where $z_1 = 1, z_2 = z_3 = p \in \mathbb{R}, 0 \leq p \leq \frac{1}{4}$, solves problem (2.1).

In the following when we refer to minimum problem (2.1) we assume that the norm in (2.1) is the Frobenius norm. Also, the symbol J is used to denote the reversion matrix $[J]_{ij} = \delta_{i,n+1-j}, i, j = 1, \dots, n$.

The uniqueness result in Theorem 2.2 implies that possible symmetries of A are inherited by its best l.s. fit \mathcal{L}_A under suitable assumptions on \mathcal{L} , as is stated in the following proposition (Proposition 2.3). Proposition 2.3 will be especially useful in Section 3 for comparing best l.s. fits from different spaces \mathcal{L} .

Proposition 2.3. *The following implications hold:*

- (i) $X^T \in \mathcal{L} \forall X \in \mathcal{L}$ (\mathcal{L} closed under transposition), $A^T = \pm A \Rightarrow \mathcal{L}_A^T = \pm \mathcal{L}_A$;
- (ii) $JX^T J \in \mathcal{L} \forall X \in \mathcal{L}$ (\mathcal{L} closed under transposition through the secondary diagonal), $A^T = \pm J A J \Rightarrow \mathcal{L}_A^T = \pm J \mathcal{L}_A J$;
- (iii) $X^H \in \mathcal{L} \forall X \in \mathcal{L}$ (\mathcal{L} closed under conjugate transposition), $A^H = \pm A \Rightarrow \mathcal{L}_A^H = \pm \mathcal{L}_A$.

Proof. Use the equalities $\|\mathcal{L}_A^T - A^T\|_F = \|\mathcal{L}_A - A\|_F = \|\mathcal{L}_A^H - A^H\|_F$. In particular, if $A = A^T$, we have $\|\mathcal{L}_A^T - A\|_F = \|\mathcal{L}_A - A\|_F$. This identity implies $\mathcal{L}_A^T = \mathcal{L}_A$ because $\mathcal{L}_A^T \in \mathcal{L}$. The remaining assertions follow from analogous arguments. \square

The following definition is essential in the general approach, here developed, concerning the best fitting and its possible applications. The main application considered in this paper regards the preconditioning technique in CG methods. Other applications, in iterative methods for minimum problems have been investigated in [22].

Definition 1. Define a space of class \mathbb{V} , a space \mathcal{L} of dimension n such that there exists $\mathbf{v} \in \mathbb{C}^n$ satisfying $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $k = 1, \dots, n$, for n matrices $J_k \in \mathcal{L}$.

As the J_k 's span \mathcal{L} , the conditions $\mathbf{v}^T J'_k = \mathbf{e}_k^T$, $J'_k \in \mathcal{L}$ imply $J'_k = J_k \forall k$, and thus the matrices J_k are uniquely determined. The matrix $\mathcal{L}_{\mathbf{v}}(\mathbf{z}) = \sum_{k=1}^n z_k J_k$ for which $\mathbf{v}^T \mathcal{L}_{\mathbf{v}}(\mathbf{z}) = \mathbf{z}^T$ is referred to as “the matrix of \mathcal{L} whose \mathbf{v} -row is $\mathbf{z}^T = [z_1 z_2 \dots z_n]$ ” (notice that two matrices of \mathcal{L} with the same \mathbf{v} -row are equal). In particular, $\mathcal{L}_{\mathbf{v}}(\mathbf{e}_k) = J_k$. If \mathbf{v} is one of the vectors of the canonical basis of \mathbb{C}^n , say \mathbf{e}_h , then \mathcal{L} is called h -space as in [3,21] and $\mathcal{L}_h(\mathbf{z}) \equiv \mathcal{L}_{\mathbf{e}_h}(\mathbf{z})$ is just the matrix of \mathcal{L} whose h th row is \mathbf{z}^T .

In more intuitive terms, in a space of class \mathbb{V} , the generic matrix is determined by a linear combination of its rows, whereas only one row (the row h) is sufficient to define the generic matrix of a h -space.

The HAs and the group matrix algebras considered, respectively, in [23] and [25] in displacement decompositions of Toeplitz-like matrices, are 1-spaces, and therefore they are subclasses of \mathbb{V} (for other examples of 1-spaces see [3]). Also the space \mathcal{L} of all symmetric Toeplitz matrices, which is not a matrix algebra, is a 1-space and therefore $\mathcal{L} \in \mathbb{V}$.

There are spaces of \mathbb{V} which are not h -spaces for any value of h . One example is the algebra γ introduced in Section 3 (see formula (3.19)). A simple example is the set of all diagonal matrices $d(\mathbf{z}) = \text{diag}(z_i, i = 1, \dots, n)$, $\mathbf{z} \in \mathbb{C}^n$. In fact $[1 \ 1 \ \dots \ 1]d(\mathbf{e}_k) = \mathbf{e}_k^T$, $k = 1, \dots, n$, while the conditions $\mathbf{e}_h^T d(\mathbf{z}_k) = \mathbf{e}_k^T$, $\mathbf{z}_k \in \mathbb{C}^n$, $k = 1, \dots, n$, cannot be verified. Both γ and $\{d(\mathbf{z}): \mathbf{z} \in \mathbb{C}^n\}$ are spaces of matrices simultaneously diagonalizable or *diagonal spaces* (see [9]). In the following proposition we prove that \mathbb{V} includes any diagonal space.

Proposition 2.4. If $\mathcal{L} = \{Md(\mathbf{z})M^{-1}: \mathbf{z} \in \mathbb{C}^n\}$ for a nonsingular matrix M , then $\mathcal{L} \in \mathbb{V}$. More specifically, for any fixed vector \mathbf{v} such that $[M^T \mathbf{v}]_j \neq 0 \forall j$, the matrix $\mathcal{L}_{\mathbf{v}}(\mathbf{z})$ is well defined and can be represented as

$$\mathcal{L}_{\mathbf{v}}(\mathbf{z}) = Md(M^T \mathbf{z})d(M^T \mathbf{v})^{-1}M^{-1}. \quad (2.9)$$

Moreover, \mathcal{L} is a h -space iff $[M]_{hj} \neq 0 \forall j$.

Proof. The matrices $J_k \equiv Md(M^T \mathbf{e}_k)d(M^T \mathbf{v})^{-1}M^{-1}$, $k = 1, \dots, n$, belong to \mathcal{L} , satisfy the identities $\mathbf{v}^T J_k = \mathbf{v}^T Md(M^T \mathbf{e}_k)d(M^T \mathbf{v})^{-1}M^{-1} = \mathbf{e}_k^T Md(M^T \mathbf{v})d(M^T \mathbf{v})^{-1}M^{-1} = \mathbf{e}_k^T$, $k = 1, \dots, n$, and span \mathcal{L} . For the last assertion in Proposition 2.4, notice that if \mathcal{L} is a h -space, then $\exists \mathbf{z}_k \in \mathbb{C}^n$ such that

$\mathbf{e}_k^T = \mathbf{e}_h^T M d(\mathbf{z}_k) M^{-1} = \mathbf{z}_k^T d(M^T \mathbf{e}_h) M^{-1}$, $k = 1, \dots, n$, and thus $d(M^T \mathbf{e}_h)$ must be nonsingular. \square

Another simple example of space of \mathbb{V} which is not a h -space for any value of h is obtained by considering the set \mathcal{L} of all the polynomials in the matrix

$$X = \begin{pmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \delta \end{pmatrix}, \quad \lambda \neq \delta, \quad \lambda, \delta \in \mathbb{C}.$$

Clearly, one is not able to define at least one of the matrices $\mathcal{L}_h(\mathbf{e}_k)$, $k = 1, 2, 3$, while, for $\mathbf{v} = [1 \ 0 \ 1]^T$, all the matrices $J_k = \mathcal{L}_{\mathbf{v}}(\mathbf{e}_k)$ are well defined (see proof of Theorem 2.5).

More generally, let X be $n \times n$ matrix with complex entries and consider the space $\{p(X)\}$ of polynomials $p(X)$ in X with complex coefficients. As the spaces of \mathbb{V} are of dimension n , a necessary condition for $\{p(X)\}$ to belong to \mathbb{V} is that X is *nonderogatory*, i.e., the minimum and the characteristic polynomials of X are equal. In the following theorem (Theorem 2.5), it is shown that this is also a sufficient condition for $\{p(X)\} \in \mathbb{V}$. Thus, Theorem 2.5 gives a new characterization of the concept of nonderogatoriness in terms of the class \mathbb{V} .

Theorem 2.5. *X is nonderogatory if and only if $\{p(X)\} \in \mathbb{V}$.*

Proof. Let us first state the following fact:

$$\{p(X)\} \in \mathbb{V}, \quad M \text{ nonsingular} \quad \Rightarrow \quad \{p(MXM^{-1})\} \in \mathbb{V}. \quad (2.10)$$

By the assumption there exist n polynomials $p^{(1)}, \dots, p^{(n)}$ and $\mathbf{v} \in \mathbb{C}^n$ such that $\mathbf{v}^T p^{(k)}(X) = \mathbf{e}_k^T$, $k = 1, \dots, n$. Let $z_k^{(j)} \in \mathbb{C}$ be such that $\sum_{k=1}^n z_k^{(j)} \mathbf{e}_k^T M^{-1} = \mathbf{e}_j^T$. Then the equalities $\mathbf{v}^T M^{-1} [\sum_{k=1}^n z_k^{(j)} p^{(k)}(MXM^{-1})] = \mathbf{e}_j^T$, $j = 1, \dots, n$, show that $\{p(MXM^{-1})\} \in \mathbb{V}$.

Now let r, n_1, \dots, n_r be arbitrary positive integers such that $\sum_{i=1}^r n_i = n$, and let $\lambda_1, \dots, \lambda_r$ be arbitrary *distinct* complex numbers. Set

$$Y_i = \left(\begin{array}{cccc} \lambda_i & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & \lambda_i \end{array} \right) \Bigg\} n_i.$$

We now prove Theorem 2.5 for $X = Y = Y_1 \oplus Y_2 \oplus \dots \oplus Y_r$. The result for generic nonderogatory matrices X will follow from (2.10) [41].

Let $i \in \{1, 2, \dots, r\}$. We want to show that there exist n_i polynomials $p_{k-1}^{(i)}(x) = \sum_{s=0}^{k-1} \alpha_s^{(i)} x^s$, $k = 1, \dots, n_i$, such that

$$\begin{aligned}
& \left(\sum_{s=1}^r \mathbf{e}_{n_1+\dots+n_{s-1}+1} \right)^T (Y - \lambda_i I)^{n_i-k} p_{k-1}^{(i)}(Y - \lambda_i I) \prod_{\substack{j=1 \\ j \neq i}}^r (Y - \lambda_j I)^{n_j} \\
&= \mathbf{e}_{n_1+\dots+n_i-k+1}^T, \quad k = 1, \dots, n_i.
\end{aligned} \tag{2.11}$$

As a consequence we shall have that $\{p(Y)\} \in \mathbb{V}$. As $\mathbf{e}_{n_1+\dots+n_{s-1}+1}^T (Y - \lambda_s I)^{n_s} = \mathbf{0}^T$, the row vector on the left-hand side in (2.11) becomes

$$\begin{aligned}
& \mathbf{e}_{n_1+\dots+n_{i-1}+1}^T (Y - \lambda_i I)^{n_i-k} p_{k-1}^{(i)}(Y - \lambda_i I) \prod_{\substack{j=1 \\ j \neq i}}^r (Y - \lambda_j I)^{n_j} \\
&= \mathbf{e}_{n_1+\dots+n_i+1-k}^T \left(\sum_{s=0}^{k-1} \alpha_s^{(i)} (Y - \lambda_i I)^s \right) \prod_{\substack{j=1 \\ j \neq i}}^r (Y - \lambda_j I)^{n_j} \\
&= [\mathbf{0}_{n_1}^T \dots \mathbf{0}_{n_{i-1}}^T \mathbf{v}_{n_i}^T \mathbf{0}_{n_{i+1}}^T \dots \mathbf{0}_{n_r}^T],
\end{aligned}$$

where $\mathbf{0}_k$ is the null vector of dimension k and \mathbf{v}_{n_i} is the n_i -vector

$$\mathbf{v}_{n_i}^T = \begin{bmatrix} 0 \dots 0 & \alpha_0^{(i)} & \alpha_1^{(i)} & \dots & \alpha_{k-1}^{(i)} \end{bmatrix} \prod_{\substack{j=1 \\ j \neq i}}^r (Y_i - \lambda_j I)^{n_j}.$$

Thus, if $\mathbf{e}_r^{(s)}$ denote the vectors of the canonical basis of \mathbb{C}^S , then (2.11) reduces to the identities $\mathbf{v}_{n_i} = \mathbf{e}_{n_i-k+1}^{(n_i)}$, $k = 1, \dots, n_i$, which are solved by choosing

$$[\alpha_0^{(i)} \alpha_1^{(i)} \dots \alpha_{k-1}^{(i)}] = \frac{1}{\beta_i} (\mathbf{e}_1^{(k)})^T \prod_{\substack{j=1 \\ j \neq i}}^r \begin{pmatrix} 1 & \frac{1}{\lambda_j - \lambda_i} & \dots & \left(\frac{1}{\lambda_j - \lambda_i} \right)^{k-1} \\ & \ddots & \ddots & \vdots \\ & & \ddots & \frac{1}{\lambda_j - \lambda_i} \\ 0 & & & 1 \end{pmatrix}^{n_j}, \tag{2.12}$$

where

$$\beta_i = \prod_{\substack{j=1 \\ j \neq i}}^r (\lambda_i - \lambda_j)^{n_j}. \quad \square$$

The class \mathbb{V} does not include any n -dimensional subspace \mathcal{L} of $M_n(\mathbb{C})$. For example, in case all the matrices of \mathcal{L} have the null vector as j th column, there is no

matrix $X \in \mathcal{L}$ and no vector \mathbf{v} such that $\mathbf{v}^T X = \mathbf{e}_j^T$ (i.e., the matrix $\mathcal{L}_{\mathbf{v}}(\mathbf{e}_j)$ is not defined).

In order to simplify the analysis of the best l.s. fit \mathcal{L}_A to A from a space \mathcal{L} of class \mathbb{V} it is useful to list in a proposition some algebraic properties of \mathbb{V} .

Proposition 2.6. *Let $\mathcal{L} \in \mathbb{V}$. Let $\mathbf{v} \in \mathbb{C}^n$ and $J_k \in \mathcal{L}$ be such that $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $k = 1, \dots, n$. Denote by P_k the $n \times n$ matrices related to the J_k by the identities $\mathbf{e}_i^T P_k = \mathbf{e}_k^T J_i$ (or $[P_k]_{ij} = [J_i]_{kj}$), $1 \leq i, k \leq n$. Then:*

- (i) $J_i X \in \mathcal{L}$, $X \in M_n(\mathbb{C}) \Rightarrow J_i X = \sum_{k=1}^n [X]_{ik} J_k$.
- (ii) \mathcal{L} is closed (under matrix multiplication) iff

$$J_i J_j = \sum_{k=1}^n [J_j]_{ik} J_k, \quad 1 \leq i, j \leq n, \quad (2.13)$$

iff $J_i P_k = P_k J_i$, $1 \leq i, k \leq n$.

- (iii) If \mathcal{L} is closed, then $\mathcal{L}_{\mathbf{v}}(\mathcal{L}_{\mathbf{v}}(\mathbf{z})^T \mathbf{z}') = \mathcal{L}_{\mathbf{v}}(\mathbf{z}') \mathcal{L}_{\mathbf{v}}(\mathbf{z})$, $\mathbf{z}, \mathbf{z}' \in \mathbb{C}^n$.
- (iv) If $I \in \mathcal{L}$ ($\mathcal{L}_{\mathbf{v}}(\mathbf{v}) = I$) and \mathcal{L} is closed, then $X \in \mathcal{L}$ is nonsingular iff $\exists \mathbf{z} \in \mathbb{C}^n$ such that $\mathbf{z}^T X = \mathbf{v}^T$; in this case $X^{-1} = \mathcal{L}_{\mathbf{v}}(\mathbf{z})$.
- (v) If \mathcal{L} is commutative, then $\mathbf{e}_i^T J_j = \mathbf{e}_j^T J_i$ (or $[J_j]_{ik} = [J_i]_{jk}$), $1 \leq i, j \leq n$, $J_i = P_i$, $1 \leq i \leq n$, $\mathbf{z}^T \mathcal{L}_{\mathbf{v}}(\mathbf{z}') = \mathbf{z}'^T \mathcal{L}_{\mathbf{v}}(\mathbf{z})$, $\mathbf{z}, \mathbf{z}' \in \mathbb{C}^n$, $I \in \mathcal{L}$ and \mathcal{L} is closed.

Proof. (i) Inspect the \mathbf{v} -row of the equality $J_i X = \sum_{k=1}^n z_k J_k$, which must hold for some $z_k \in \mathbb{C}$.

(ii) Eq. (2.13) is a simple consequence of (i) for $X = J_j$. The equality $J_i P_k = P_k J_i$ follows by writing the element (r, s) of (2.13).

(iii) The matrices $\mathcal{L}_{\mathbf{v}}(\mathcal{L}_{\mathbf{v}}(\mathbf{z})^T \mathbf{z}')$ and $\mathcal{L}_{\mathbf{v}}(\mathbf{z}') \mathcal{L}_{\mathbf{v}}(\mathbf{z})$ are in \mathcal{L} and have the same \mathbf{v} -row.

(iv) Calculate, by (ii), $\mathbf{e}_k^T \mathcal{L}_{\mathbf{v}}(\mathbf{z}) X = \mathbf{z}^T P_k X = \mathbf{z}^T X P_k = \mathbf{v}^T P_k = \mathbf{e}_k^T$.

(v) Observe that $\mathbf{e}_i^T J_j = \mathbf{v}^T J_i J_j = \mathbf{v}^T J_j J_i = \mathbf{e}_j^T J_i$. This identity yields the remaining assertions. \square

In the following definition (Definition 2) we wish to extend, in \mathbb{V} , the class of matrices where good approximations (in Frobenius norm) to A —corresponding, in principle, to good optimal preconditioners of the linear system $A\mathbf{x} = \mathbf{b}$ —could be chosen.

Definition 2. Call \ast -space a subspace \mathcal{L} of $M_n(\mathbb{C})$ spanned by J_i , $i = 1, \dots, n$, linearly independent, subject to the following conditions:

$$I \in \mathcal{L} \quad \text{and} \quad J_i^H J_j = \sum_{k=1}^n [\overline{J_k}]_{ij} J_k, \quad 1 \leq i, j \leq n. \quad (*)$$

The equality in (*) may seem rather meaningless, but this is not really the case, because (*) denotes a common property of the following two classes of algebras \mathcal{L} :

(SDU): \mathcal{L} = space of matrices simultaneously diagonalized by a unitary transform;

(GA): \mathcal{L} = group matrix algebra.

In fact we have the following:

Proposition 2.7. *Let $\mathcal{L} \in \mathbb{V}(\mathbf{v}^T J_k = \mathbf{e}_k^T)$. Then \mathcal{L} satisfies (*) in case:*

(i) \mathcal{L} is commutative, $J_i^H \in \mathcal{L}$, or/and

(ii) \mathcal{L} is closed under matrix multiplication, $J_i^H = \alpha_i J_{t_i}$, $|\alpha_i| = 1$ and $I \in \mathcal{L}$.

Clearly, (SDU) implies (i) whereas (GA) implies (ii).

Proof. (i) By Proposition 2.6(i), (v),

$$J_i^H J_j = J_j J_i^H = \sum_{k=1}^n [J_i^H]_{jk} J_k = \sum_{k=1}^n [\overline{J_i}]_{kj} J_k = \sum_{k=1}^n [\overline{J_k}]_{ij} J_k.$$

(ii) First observe that $t_i \neq t_j$, $i \neq j$, $i, j = 1, \dots, n$. We have

$$J_i^H J_j = \alpha_i J_{t_i} J_j = \alpha_i \sum_{k=1}^n [J_j]_{t_i k} J_k = \sum_{k=1}^n \alpha_i \overline{\alpha_j} [P_k^H]_{t_i t_j} J_k. \quad (2.14)$$

Moreover,

$$J_j J_k = \sum_{i=1}^n [J_k]_{ji} J_i \Rightarrow J_{t_k} J_{t_j} = \sum_{i=1}^n \frac{\alpha_i}{\alpha_k \alpha_j} [\overline{J_k}]_{ji} J_{t_i} = \sum_{i=1}^n \frac{\alpha_i}{\alpha_j} [J_{t_k}]_{ij} J_{t_i},$$

$$J_{t_k} J_{t_j} = \sum_{i=1}^n [J_{t_j}]_{t_k t_i} J_{t_i} = \sum_{i=1}^n [P_{t_k}^T]_{t_i t_j} J_{t_i}.$$

Thus, $\overline{\alpha_j} [P_k^H]_{t_i t_j} = \overline{\alpha_i} [\overline{J_k}]_{ij}$ and, by (2.14), \mathcal{L} satisfies (*) if $|\alpha_i| = 1$. \square

Example 1. The noncommutative space \mathcal{L} spanned by the matrices

$$J_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad J_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix},$$

$$J_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad J_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

belongs to $\mathbb{V}(\mathcal{L}_1(\mathbf{e}_k) = J_k)$ and satisfies condition (ii) of Proposition 2.7, but is not a GA. Thus, GA denotes a *proper* subset of the set of spaces verifying the same condition (ii).

The following proposition states some important properties of $*$ -spaces. In particular, a $*$ -space is a space of class \mathbb{V} .

Proposition 2.8. *Let \mathcal{L} satisfy $(*)$.*

- (i) *If $I = \sum_{k=1}^n v_k J_k$, then for $\mathbf{v} = [v_1 v_2 \cdots v_n]^T$ we have $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $1 \leq k \leq n$, and thus $\mathcal{L} \in \mathbb{V}$.*
- (ii) *\mathcal{L} is closed under conjugate transposition ($J_i^H \in \mathcal{L}$).*
- (iii) *\mathcal{L} is closed under matrix multiplication.*

Proof. (i) Multiply the identity in $(*)$ by \bar{v}_i and sum upon i to obtain $J_j = \sum_{k=1}^n \mathbf{v}^H J_k \mathbf{e}_j J_k$, $1 \leq j \leq n$. Then the linear independence of the J_k implies $\mathbf{v}^T J_k = \mathbf{e}_k^T$, $1 \leq k \leq n$.

(ii) Multiply the identity in $(*)$ by v_j and sum upon j to show that $J_i^H \in \mathcal{L}$.

(iii) As the matrices J_i^H are in \mathcal{L} and are linearly independent, $J_s = \sum_{i=1}^n z_i^{(s)} J_i^H \forall s$, for some $z_i^{(s)} \in \mathbb{C}$. By multiplying the identity in $(*)$ by $z_i^{(s)}$ and summing upon i we have $J_s J_j \in \mathcal{L} \forall s, j$. \square

Example 2. The algebra C_β of β -circulant matrices spanned by $J_k = (P_\beta)^{k-1}$, $1 \leq k \leq n$, where

$$P_\beta = \begin{pmatrix} 0 & 1 & & 0 \\ \vdots & 0 & 1 & \\ 0 & & \ddots & 1 \\ \beta & 0 & \cdots & 0 \end{pmatrix}, \quad \beta \in \mathbb{C},$$

is a space of class \mathbb{V} (by choosing $(C_\beta)_1(\mathbf{e}_k) = J_k$, one realizes that C_β is a 1-space) of matrices simultaneously diagonalized by the transform

$$M = \frac{1}{\sqrt{n}} \left((\sqrt[n]{\beta})^{k-1} \omega^{(k-1)(j-1)} \right)_{k,j=1}^n, \quad \omega = \exp(-i 2\pi/n),$$

that is unitary iff $|\beta| = 1$. Moreover, if $|\beta| \neq 1$, then $J_k^H \notin C_\beta$. Thus, by Proposition 2.8(ii), C_β satisfies $(*)$ iff $|\beta| = 1$.

The following proposition and lemma are exploited in the proof of the main result of this section (Theorem 2.11) which states that the spectrum of \mathcal{L}_A is “contained” in the spectrum of A if $A = A^H$ and \mathcal{L} is a $*$ -space. Proposition 2.9 will be also used in Section 4 to solve the linear system $B_{\mathcal{L}} \mathbf{z} = \mathbf{c}_{\mathcal{L},A}$ of Theorem 2.2, and thus to calculate \mathcal{L}_A , for some special choices of \mathcal{L} .

Proposition 2.9. *Let \mathcal{L} satisfy $(*)$. Then $\bar{B}_{\mathcal{L}} \in \mathcal{L}$, in fact*

$$\bar{B}_{\mathcal{L}} = \sum_{k=1}^n P_k P_k^H = \sum_{k=1}^n (\overline{\text{tr } J_k}) P_k = \sum_{k=1}^n (\overline{\text{tr } J_k}) J_k. \quad (2.15)$$

Moreover, if \mathcal{L}_A is the best l.s. fit to $A \in M_n(\mathbb{C})$ from \mathcal{L} , then

$$\mathcal{L}_A = \mathcal{L}_{\mathbf{v}}(B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}) = \mathcal{L}_{\mathbf{v}}(\mathbf{c}_{\mathcal{L},A}) \overline{B_{\mathcal{L}}}^{-1} = \overline{B_{\mathcal{L}}}^{-1} \mathcal{L}_{\mathbf{v}}(\mathbf{c}_{\mathcal{L},A}). \quad (2.16)$$

Proof. By (2.5) the three identities in (2.15) are obtained, respectively, as follows (the first one does not require any hypothesis on \mathcal{L}):

$$\begin{aligned} [B_{\mathcal{L}}]_{ij} &= \sum_{r,t=1}^n [\overline{P_r}]_{it} [P_r]_{jt} = \sum_{r=1}^n [\overline{P_r} P_r^T]_{ij}, \\ [B_{\mathcal{L}}]_{ij} &= \sum_{r=1}^n \sum_{t=1}^n [J_j]_{rt} [J_i^H]_{tr} = \sum_{r=1}^n [J_j J_i^H]_{rr} = \sum_{k=1}^n (\text{tr } J_k) [\overline{P_k}]_{ij} \end{aligned}$$

(use Proposition 2.6(i) for $X = J_i^H$), and finally, using (*),

$$[B_{\mathcal{L}}]_{ij} = \sum_{t=1}^n \sum_{r=1}^n [J_i^H]_{tr} [J_j]_{rt} = \sum_{t=1}^n [J_i^H J_j]_{tt} = \sum_{k=1}^n (\text{tr } J_k) [\overline{J_k}]_{ij}.$$

By (2.15) and by Proposition 2.6(iv), (ii), $\overline{B_{\mathcal{L}}}$ and $\overline{B_{\mathcal{L}}}^{-1}$ are in \mathcal{L} and commute with any $X \in \mathcal{L}$. Thus, Proposition 2.6(iii) yields (2.16). \square

Example 3. Let $\mathcal{G} = \{1, 2, \dots, n\}$ be a group, let 1 be the identity element of \mathcal{G} , and set $\mathcal{L} = \mathbb{C}[\mathcal{G}] = \{X \in M_n(\mathbb{C}): x_{i,j} = x_{ki,kj}, i, j, k \in \mathcal{G}\}$. The GA \mathcal{L} is a 1-space and the matrices $J_k \equiv \mathcal{L}_1(\mathbf{e}_k)$ (for which $\mathbf{e}_1^T J_k = \mathbf{e}_k^T$) are permutation matrices such that $J_1 = I$ and, for $k \neq 1$, J_k has all diagonal entries equal to 0. Thus, by (2.15), $B_{\mathcal{L}} = nI$ and, by (2.16), $\mathcal{L}_A = \mathcal{L}_1(\mathbf{z})$, where (taking into account that $[J_k]_{i,j} = [J_k]_{1,i^{-1}j} = \delta_{j,ik}$)

$$\mathbf{z} = \frac{1}{n} \mathbf{c}_{\mathcal{L},A} = \left(\frac{\sum_{i,j=1}^n [J_k]_{ij} a_{ij}}{n} \right)_{k=1}^n = \left(\frac{\sum_{i=1}^n a_{i,ik}}{n} \right)_{k=1}^n. \quad (2.17)$$

If \mathcal{G} is cyclic ($s = g^{s-1}$, $s = 1, \dots, n$, $g^n = g^0$), then \mathcal{L} is the GA C of circulant matrices and \mathcal{L}_A is the Chan preconditioner C_A [18], whose $(1, k)$ entry is, by (2.17), $(\sum_{i=1}^{n-k+1} a_{i,i+k-1} + \sum_{i=n-k+2}^n a_{i,i+k-1-n})/n$.

If $\mathcal{L} = C_{\beta}$ (see Example 2), then, by Theorem 2.2, $B_{\mathcal{L}} = d(\mathbf{z})$, where $z_k = (k-1)|\beta|^2 + n - k + 1$, $k = 1, \dots, n$ (notice that $\overline{B_{\mathcal{L}}} \in \mathcal{L} \Leftrightarrow |\beta| = 1$), and therefore \mathcal{L}_A is the β -circulant matrix $(C_{\beta})_A$ whose $(1, k)$ entry is

$$\left(\sum_{i=1}^{n-k+1} a_{i,i+k-1} + \overline{\beta} \sum_{i=n-k+2}^n a_{i,i+k-1-n} \right) / z_k.$$

Lemma 2.10. Let \mathcal{L} satisfy (*). Then $\forall \mathbf{z} \in \mathbb{C}^n$,

$$\mathbf{z}^H \mathcal{L}_{\mathbf{v}}(\mathbf{c}_{\mathcal{L},A}) \mathbf{z} = \sum_{k=1}^n [P_k^H \mathbf{z}]^H A [P_k^H \mathbf{z}]. \quad (2.18)$$

Proof.

$$\begin{aligned}
 \mathbf{z}^H \mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})} \mathbf{z} &= \mathbf{z}^H \sum_{k=1}^n (J_k, A) J_k \mathbf{z} \\
 &= \sum_{i,j=1}^n \bar{z}_i z_j \sum_{r,t=1}^n a_{rt} \sum_{k=1}^n [J_k]_{ij} [\overline{J_k}]_{rt} \\
 &= \sum_{i,j=1}^n \bar{z}_i z_j \sum_{r,t=1}^n a_{rt} [\overline{J_i^H J_j}]_{rt} \\
 &= \sum_{r,t=1}^n a_{rt} \sum_{i,j=1}^n \bar{z}_i z_j \sum_{k=1}^n [\overline{J_i^H}]_{rt} [\overline{J_j}]_{kt} \\
 &= \sum_{k=1}^n \sum_{r,t=1}^n a_{rt} \left(\sum_{i=1}^n \bar{z}_i [P_k^H]_{ri} \right) \left(\sum_{j=1}^n z_j [P_k]_{tj} \right). \quad \square
 \end{aligned}$$

For a Hermitian matrix A , Lemma 2.10 and the first identity in (2.15) yield

$$\min \lambda(A) \leq \frac{\mathbf{z}^H \mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})} \mathbf{z}}{\mathbf{z}^H \overline{B}_{\mathcal{L}} \mathbf{z}} \leq \max \lambda(A) \quad \forall \mathbf{z} \in \mathbb{C}^n, \quad (2.19)$$

where $\lambda(A)$ is the generic eigenvalue of A . If the J_k 's in (*) satisfy the “orthonormality” condition $(J_i, J_j) = \delta_{i,j}$ (as for the case of \mathcal{L} = group matrix algebra), then

$$\frac{\mathbf{z}^H \mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})} \mathbf{z}}{\mathbf{z}^H \overline{B}_{\mathcal{L}} \mathbf{z}} = \frac{\mathbf{z}^H \mathcal{L}_A \mathbf{z}}{\mathbf{z}^H \mathbf{z}},$$

and therefore (2.19) lets us conclude that the eigenvalues of \mathcal{L}_A are in the interval $[\min \lambda(A), \max \lambda(A)]$. However, as it is shown in the following theorem (Theorem 2.11), the orthonormality condition is not necessary to prove this result. In Theorem 2.11, for a real matrix X , X_s denotes the matrix $\frac{1}{2}(X + X^T)$, the symmetric part of X .

Theorem 2.11. *Let \mathcal{L} be a subspace of $M_n(\mathbb{C})$ satisfying (*). Let $A \in M_n(\mathbb{C})$ and let \mathcal{L}_A be the best l.s. fit to A from \mathcal{L} .*

- (i) *If $A = A^H$, then $\mathcal{L}_A = \mathcal{L}_A^H$ and $\min \lambda(A) \leq \lambda(\mathcal{L}_A) \leq \max \lambda(A)$. As a consequence \mathcal{L}_A is positive definite if A is positive definite.*
- (ii) *If A is real, then $\min \lambda(A_s) \leq \operatorname{Re} \lambda(\mathcal{L}_A) \leq \max \lambda(A_s)$. Moreover, if the J_k in (*) are real (in this case \mathcal{L}_A is real), $(\mathcal{L}_A)_s$ is positive definite if A_s is positive definite.*

Proof. Let M be a Hermitian matrix such that $M^2 = \overline{B}_{\mathcal{L}}^{-1}$ and consider the matrix $M\mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})}M$. As a consequence of (2.16), $M\mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})}M$ is similar to \mathcal{L}_A . Then $\lambda(\mathcal{L}_A)$ is an eigenvalue of $M\mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})}M$, i.e., $\exists \mathbf{x} \in \mathbb{C}^n$ with $\|\mathbf{x}\|_2 = 1$ such that $\lambda(\mathcal{L}_A) = \mathbf{x}^H M\mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})}M\mathbf{x}$; thus, by Lemma 2.10,

$$\lambda(\mathcal{L}_A) = \sum_{k=1}^n \mathbf{x}_k^H A \mathbf{x}_k, \quad \mathbf{x}_k = P_k^H M \mathbf{x}. \quad (2.20)$$

Notice that the first identity in (2.15) implies

$$\sum_{k=1}^n \mathbf{x}_k^H \mathbf{x}_k = 1 = \sum_{k=1}^n [(\operatorname{Re} \mathbf{x}_k)^T (\operatorname{Re} \mathbf{x}_k) + (\operatorname{Im} \mathbf{x}_k)^T (\operatorname{Im} \mathbf{x}_k)].$$

This remark and (2.20) yield the inequalities in (i) and (ii). Moreover, if $A = A^H$, then, by Proposition 2.3(iii), $\mathcal{L}_A = \mathcal{L}_A^H$. Now assume that A and the J_k are real, and that $\mathbf{z}^T A \mathbf{z} > 0 \forall \mathbf{z} \in \mathbb{R}^n, \mathbf{z} \neq 0$. Then the matrix M can be chosen real and, by Lemma 2.10, we have

$$\mathbf{z}^T M \mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})} M \mathbf{z} = \sum_{k=1}^n [P_k^T M \mathbf{z}]^T A [P_k^T M \mathbf{z}] \quad \forall \mathbf{z} \in \mathbb{R}^n.$$

This identity implies that the matrix $(\mathcal{L}_A)_s$ is positive definite because, by (2.16), $(\mathcal{L}_A)_s = M(M\mathcal{L}_{\mathbf{v}(\mathbf{c}_{\mathcal{L},A})}M)_s M^{-1}$. \square

One can obtain assertions (i) and (ii) of Theorem 2.11 in the more specific case where $\mathcal{L} = \{Ud(\mathbf{z})U^H: \mathbf{z} \in \mathbb{C}^n\}$, with U = unitary matrix, by using the identities $\mathbf{u}_k^H \mathcal{L}_A \mathbf{u}_k = \mathbf{u}_k^H A \mathbf{u}_k$, $\mathbf{u}_k = U \mathbf{e}_k$. These identities, which were first derived for $\mathcal{L} = C$ [38], follow from the equality

$$\mathcal{L}_A = U \operatorname{diag}([U^H A U]_{kk}, k = 1, \dots, n) U^H \quad (2.21)$$

found in [14,28] as a simple consequence of the fact that $\|\cdot\|_F$ is unitary invariant (see also [33] and the references therein). In Theorem 2.11, it is proved that, in order to obtain properties like (i) and/or (ii) is not really necessary, as one may guess on the basis of the known literature, that \mathcal{L} is a space of matrices simultaneously diagonalizable by a unitary transform.

In Sections 3–6, we mainly deal with matrix algebras \mathcal{L} that are 1-spaces, and therefore the results of the present section are used for $\mathbf{v} = \mathbf{e}_1$. Then take into account that, from now on, $\mathcal{L}_1(\mathbf{z})$ and $J_k = \mathcal{L}_1(\mathbf{e}_k)$, the matrices of \mathcal{L} with first row \mathbf{z}^T and \mathbf{e}_k^T , respectively, are simply denoted by $\mathcal{L}(\mathbf{z})$ and $J_k = \mathcal{L}(\mathbf{e}_k)$.

3. Matrix algebras close to symmetric Toeplitz matrices: μ , η , \mathcal{K} , \mathcal{H} , γ

For particular choices of A and \mathcal{L} , matrices \mathcal{L}_A solving problem (2.1) have been exploited to precondition linear systems $A\mathbf{x} = \mathbf{b}$. Such matrices are therefore generally called *optimal* preconditioners. In particular, in the important case where A

is a symmetric Toeplitz matrix, $A = T = (t_{|i-j|})_{i,j=1}^n$, the fit \mathcal{L}_T is known to be an efficient preconditioner of $T\mathbf{x} = \mathbf{b}$ for at least four different algebras \mathcal{L} : the algebras C and C_{-1} of circulant [18] and (-1) -circulant [27] matrices, the algebra τ [6,9,16], and the Hartely algebra \mathcal{H} [8,30] (see also [31]). In this section, we consider other four examples of matrix algebras closely related to symmetric Toeplitz matrices: μ , η , \mathcal{H} and γ . Three of these algebras, μ , η and \mathcal{H} , have been introduced in the context of displacement formulas for Toeplitz plus Hankel-like matrices [20,21]. We shall see that they also yield very good fits to T (see Theorem 3.6) which turn out to be optimal preconditioners competitive with the best known (Theorem 5.1). Moreover, in Corollary 3.7, η and μ are used to define two new fits to a *Hermitian* Toeplitz matrix. A fourth algebra γ , strictly related to μ , is introduced in this paper. Matrices from each of the algebras η , μ and γ are shown to be simultaneously diagonalized by a fast *real* transform (in [21] only complex transforms diagonalizing η and μ are found). As most of the algebras \mathcal{L} considered in this section are $*$ -spaces, both Proposition 2.9 and Theorem 2.11 hold.

Let P_β be the $n \times n$ matrix

$$P_\beta = \begin{pmatrix} 0 & 1 & & & 0 \\ \vdots & 0 & & 1 & \\ \vdots & & \ddots & & \ddots \\ 0 & & & \ddots & 1 \\ \beta & 0 & & \dots & 0 \end{pmatrix}, \quad \beta \in \mathbb{C}, \quad (3.1)$$

and denote by C_β the matrix algebra generated by P_β . Then the generic matrix of C_β is $C_\beta(\mathbf{z}) = \sum_{k=1}^n z_k J_k$, $J_k = P_\beta^{k-1}$. For $\beta = 1$ and $\beta = -1$ one obtains, respectively, the circulant ($C = C_1$) and the (-1) -circulant (C_{-1}) matrices. For $\beta = \pm 1$, set

$$C_\beta^S = \{A \in C_\beta: A^T = A\} \quad \text{and} \quad C_\beta^{SK} = \{A \in C_\beta: A^T = -A\}. \quad (3.2)$$

The space C_β^S is the algebra of *symmetric* β -circulant matrices, and C_β^{SK} is the space of *skewsymmetric* β -circulant matrices.

The algebras μ , η and \mathcal{H} are defined as follows [21]:

$$\mu = C_{-1}^S + J C_{-1}^S, \quad \eta = C^S + J C^S, \quad \mathcal{H} = C_{-1}^S + J P_{-1} C_{-1}^{SK}. \quad (3.3)$$

Notice that μ is the (-1) -circulant version of η , and that \mathcal{H} is the (-1) -circulant version of the “Hartley” algebra $\mathcal{H} = C^S + J P_1 C^{SK}$ introduced in [8]. One can easily realize that the spaces μ , η , \mathcal{H} and \mathcal{H} are effectively algebras, i.e., they are closed under matrix multiplication, and that matrices from \mathcal{H} and \mathcal{H} are symmetric, while matrices from μ and η are simultaneously symmetric and persymmetric.

Denote by τ the matrix algebra generated by $X = P_0 + P_0^T$. Then the generic element of τ is $\tau(\mathbf{z}) = \sum_{k=1}^n z_k J_k$, where $J_1 = I$, $J_2 = X$ and $J_k = J_{k-1}X - J_{k-2}$, $k = 3, \dots, n$. For $\mathbf{z} \in \mathbb{C}^n$ set $I_2^{n-1}\mathbf{z} = [z_{n-1} \cdots z_2]^T$, $I_2^n\mathbf{z} = [z_n \cdots z_2]^T$ and $\mathbf{e}_k^{(n-1)}$

$= I_2^n \mathbf{e}_{n-k+1}$, $k = 1, \dots, n-1$. Let $\mathcal{C}_\pm(\cdot; \mathbf{p})$ be the symmetric 1-space defined as the set of all matrices

$$\begin{aligned} \mathcal{C}_\pm(\mathbf{z}; \mathbf{p}) = \tau(\mathbf{z}) \mp & \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \tau(I_2^{n-1} \mathbf{z}) & \vdots \\ 0 & \cdots & 0 \end{pmatrix} \\ & + \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \tau(I_2^n \mathbf{z}) \tau(\mathbf{p}) & \\ 0 & & \end{pmatrix}, \quad \mathbf{z} \in \mathbb{C}^n, \end{aligned} \quad (3.4)$$

where $\mathbf{p} \in \mathbb{C}^{n-1}$ is fixed such that $J\mathbf{p} = \mp \mathbf{p}$. Set

$$T_{0,0}^{\pm 1, \pm 1} = \begin{pmatrix} 0 & 1 & & \pm 1 \\ 1 & 0 & 1 & \\ & 1 & & \ddots \\ & & \ddots & 1 \\ \pm 1 & & & 1 & 0 \end{pmatrix}. \quad (3.5)$$

Theorem 3.1 [21].

(i) The space $\mathcal{C}_\pm(\cdot; \mathbf{p})$ is closed under matrix multiplication, contains the matrix $T_{0,0}^{\pm 1, \pm 1}$ and satisfies the identity

$$\begin{aligned} \mathcal{C}_\pm(\cdot; \mathbf{p}) = \left\{ A \in M_n(\mathbb{C}) : AT_{0,0}^{\pm 1, \pm 1} = T_{0,0}^{\pm 1, \pm 1} A \right. \\ \left. \text{and } A\mathcal{C}_\pm(\mathbf{e}_n; \mathbf{p}) = \mathcal{C}_\pm(\mathbf{e}_n; \mathbf{p})A \right\}. \end{aligned} \quad (3.6)$$

(ii) If \mathcal{L} is a symmetric closed 1-space containing $T_{0,0}^{\pm 1, \pm 1}$, then $\mathcal{L} = \mathcal{C}_\pm(\cdot; \mathbf{p})$ for some $\mathbf{p} = \mp J\mathbf{p}$.

(iii) For $\mathfrak{H} = \{\mathcal{C}_+(\cdot; \mathbf{p}) : J\mathbf{p} = -\mathbf{p}\}$ and $\mathfrak{K} = \{\mathcal{C}_-(\cdot; \mathbf{p}) : J\mathbf{p} = \mathbf{p}\}$, we have $C^S \subset \mathcal{L} \subset C + JC \forall \mathcal{L} \in \mathfrak{H}$, $C_{-1}^S \subset \mathcal{L} \subset C_{-1} + JC_{-1} \forall \mathcal{L} \in \mathfrak{K}$.

(iv) $\mu, \mathcal{K} \in \mathfrak{K}$ and $\eta, \mathcal{H} \in \mathfrak{H}$ in fact

$$\begin{aligned} \mathcal{C}_-\left(\cdot; -\frac{1}{2}(\mathbf{e}_2^{(n-1)} + \mathbf{e}_{n-2}^{(n-1)})\right) &= \mathcal{K}, \\ \mathcal{C}_+\left(\cdot; \frac{1}{2}(\mathbf{e}_2^{(n-1)} - \mathbf{e}_{n-2}^{(n-1)})\right) &= \mathcal{H}, \\ \mathcal{C}_-(\cdot; \mathbf{0}) &= \mu, \\ \mathcal{C}_+(\cdot; \mathbf{0}) &= \eta. \end{aligned} \quad (3.7)$$

In particular, η , μ , \mathcal{H} , \mathcal{K} are 1-spaces. Notice that $\mathcal{C}_{\pm}(\mathbf{e}_n; \mathbf{0}) = J$, thus $\mu(\eta)$ is the only algebra of $\mathfrak{K}(\mathfrak{H})$ which is also persymmetric.

From (3.7) and (3.6) we obtain, as for the algebra τ , a *cross-sum* structure for both η and μ :

Proposition 3.2. Let $A = (a_{ij})_{i,j=1}^n$ be a matrix from $\tau(\eta) [\mu]$. Then

$$a_{i,j-1} + a_{i,j+1} = a_{i-1,j} + a_{i+1,j}, \quad 1 \leq i, j \leq n, \quad (3.8)$$

where $a_{0,n+1-k} = a_{n+1,k} = a_{n+1-k,0} = a_{k,n+1} = 0$ ($a_{1,k}$) $[-a_{1,k}]$, $k = 1, \dots, n$.

By Proposition 3.2 and by the identities $A^T = A = JAJ$ one can easily write down the matrix A of $\tau(\eta) [\mu]$ whose first row is $\{z_1 z_2 \cdots z_n\}$.

For example, for $n = 8$ one calculates

$$\begin{aligned} \tau(\mathbf{e}_3) &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ & 1 & & & & & & \\ & 1 & & 1 & & & & \\ 1 & & 1 & & 1 & & & \\ & 1 & & 1 & & 1 & & \\ & & 1 & & 1 & & 1 & \\ & & & 1 & & 1 & & 1 \\ & & & & 1 & & 1 & \\ & & & & & 1 & & \end{pmatrix}, \\ \eta(\mathbf{e}_3) &= \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & & \\ & 1 & & & & & & \\ & 1 & & 1 & -1 & & & \\ 1 & & 1 & & 0 & & -1 & \\ & 1 & & 0 & & 0 & & \\ & & 0 & & 0 & & 1 & \\ -1 & & & 0 & & 1 & & 1 \\ & -1 & & 1 & & 1 & & \\ & & & & 1 & & & \end{pmatrix}, \\ \mu(\mathbf{e}_3) &= \begin{pmatrix} 0 & 0 & 0 & 0 & -1 & 0 & & \\ & 1 & & & & & & \\ & 1 & & 1 & & 1 & & \\ 1 & & 1 & & 2 & & 1 & \\ & 1 & & 2 & & 2 & & \\ & & 2 & & 2 & & 1 & \\ 1 & & 2 & & 1 & & 1 & \\ & 1 & & 1 & & 1 & & \\ & & & & 1 & & & \end{pmatrix}. \end{aligned}$$

The interest of μ , η , \mathcal{K} and \mathcal{H} , with respect to other algebras from \mathfrak{H} or \mathfrak{K} , is mainly justified by the fact that for $\mathcal{L} \in \{\mu, \eta, \mathcal{K}, \mathcal{H}\}$ a *real* fast transform $Q_{\mathcal{L}}$ diagonalizing all matrices of \mathcal{L} can be effectively defined. This result, stated in the following theorem (Theorem 3.3), is new for $\mathcal{L} \in \{\mu, \eta\}$. Just Theorem 3.3 where the matrices Q_{μ} , Q_{η} , $Q_{\mathcal{K}}$ and $Q_{\mathcal{H}}$ are displayed, leads to the definition of a new orthonormal $n \times n$ matrix G such that $G\mathbf{z}$ is a fast transform and the space γ of all matrices diagonalised by G is (for $n \neq 2 + 4r$) an algebra of \mathfrak{K} *different* from μ and \mathcal{K} .

Theorem 3.3. *Let $\mathcal{L} \in \{\mu, \eta, \mathcal{K}, \mathcal{H}\}$. Then, for all $\mathbf{z} \in \mathbb{C}^n$,*

$$\mathcal{L}(\mathbf{z}) = Q_{\mathcal{L}} d(Q_{\mathcal{L}}^T \mathbf{z}) d(Q_{\mathcal{L}}^T \mathbf{e}_1)^{-1} Q_{\mathcal{L}}^T, \quad (3.9)$$

where $Q_{\mathcal{L}}$ is the orthonormal matrix

$$[Q_{\mathcal{H}}]_{kj} = \frac{1}{\sqrt{n}} \left(\cos \frac{2\pi(k-1)(j-1)}{n} \pm \sin \frac{2\pi(k-1)(j-1)}{n} \right),$$

$$k, j = 1, \dots, n, \quad (3.10)$$

$$[Q_{\mathcal{K}}]_{kj} = \frac{1}{\sqrt{n}} \left(\cos \frac{\pi(k-1)(2j-1)}{n} \pm \sin \frac{\pi(k-1)(2j-1)}{n} \right),$$

$$k, j = 1, \dots, n, \quad (3.11)$$

$$[Q_{\eta}]_{kj} = \begin{cases} 1/\sqrt{n}, & j = 1, \\ \sqrt{2/n} \cos \frac{\pi(2k-1)(j-1)}{n}, & j = 2, \dots, \lceil \frac{1}{2}n \rceil, \\ (-1)^{k-1}/\sqrt{n}, & j = \frac{1}{2}n + 1 \text{ (} n \text{ even)}, \\ \sqrt{2/n} \sin \frac{\pi(2k-1)(j-1)}{n} & j = \lfloor \frac{1}{2}n + 2 \rfloor, \dots, n, \\ & k = 1, \dots, n, \end{cases} \quad (3.12)$$

$$[Q_{\mu}]_{kj} = \begin{cases} \sqrt{2/n} \sin \frac{\pi(2k-1)(2j-1)}{2n}, & j = 1, \dots, \lceil \frac{1}{2}(n-1) \rceil, \\ (-1)^{k-1}/\sqrt{n}, & j = \frac{1}{2}(n+1) \text{ (} n \text{ odd)}, \\ \sqrt{2/n} \cos \frac{\pi(2k-1)(2j-1)}{2n} & j = \lfloor \frac{1}{2}(n+3) \rfloor, \dots, n, \\ & k = 1, \dots, n. \end{cases} \quad (3.13)$$

Proof. For the cases $\mathcal{L} = \mathcal{H}$ and $\mathcal{L} = \mathcal{K}$ see, respectively, [8] and [21]. Assume that $\mathcal{L} \in \{\mu, \eta\}$. Set $\rho = \exp(-i\pi/n)$, $\omega = \rho^2$, $[F]_{ij} = (1/\sqrt{n})\omega^{(i-1)(j-1)}$, $i, j = 1, \dots, n$, $D_{\rho} = \text{diag}(\rho^{k-1}, k = 1, \dots, n)$. In [21], it is shown that, for all $\mathbf{z} \in \mathbb{C}^n$, $\mathcal{L}(\mathbf{z}) = M_{\mathcal{L}} d(M_{\mathcal{L}}^T \mathbf{z}) d(M_{\mathcal{L}}^T \mathbf{e}_1)^{-1} M_{\mathcal{L}}^H$, where $M_{\mathcal{L}}$ is the unitary matrix dis-

played below. In the definition of M_η (M_μ) the central row and column including $\sqrt{2}$ are absent in case n odd (n even):

$$M_\eta = \frac{1}{\sqrt{2}} F \begin{pmatrix} \sqrt{2} & 0 & & & & & 0 \\ 0 & 1 & & & & & -\omega \\ & & 0 & & & & -\omega^2 \\ & & & \ddots & & & \\ & & & & 1 & -\omega^k & \\ & 0 & & & \sqrt{2} & & 0 \\ & & & \omega^{n-k} & 1 & & \\ & & & & & \ddots & \\ & & \omega^{n-2} & & & & \\ 0 & \omega^{n-1} & & 0 & & & 1 \end{pmatrix},$$

$$k = \left\lceil \frac{n}{2} - 1 \right\rceil, \quad (3.14)$$

$$M_\mu = \frac{1}{\sqrt{2}} D_\rho F \begin{pmatrix} 1 & & & & & & \rho \\ & \ddots & & 0 & & & \rho^3 \\ & & 1 & & \rho^k & & \\ 0 & & & \sqrt{2} & & 0 & \\ & \rho^{n-k} & & 1 & & & \\ & & \ddots & & & \ddots & \\ \rho^{n-3} & & & 0 & & & \\ \rho^{n-1} & & & & & & 1 \end{pmatrix},$$

$$k = 2 \left\lfloor \frac{n}{2} \right\rfloor - 1. \quad (3.15)$$

Now observe that a diagonal matrix D can be chosen in such a way that $M_\mathcal{Q} D$ is (unitary and) real. The matrix $Q_\mathcal{Q}$ (see (3.12) and (3.13)) is precisely the matrix $M_\mathcal{Q} D_\mathcal{Q}$, where

$$[D_\eta]_{kk} = \begin{cases} \omega^{(k-1)/2}, & k = 1, \dots, \lceil \frac{1}{2}n \rceil, \\ i\omega^{(k-1)/2}, & k = \lceil \frac{1}{2}n + 1 \rceil, \dots, n, \end{cases}$$

$$[D_\mu]_{kk} = \begin{cases} i\rho^{(2k-1)/2}, & k = 1, \dots, \lceil \frac{1}{2}n \rceil, \\ \rho^{(2k-1)/2}, & k = \lceil \frac{1}{2}n + 1 \rceil, \dots, n. \end{cases} \quad \square$$

The matrix Q_η in (3.12) is related to the matrix $Q_{\mathcal{H}}$ in (3.11) by the identity

$$\sqrt{2}Q_{\mathcal{H}}^T = Q_\eta \begin{pmatrix} \sqrt{2} & & & \\ & I & & -J \\ & & \pm\sqrt{2} & \\ \pm J & & & \pm I \end{pmatrix}, \quad I = I_{\lfloor (n-1)/2 \rfloor}, \quad (3.16)$$

where the central row and column including $\pm\sqrt{2}$ are absent in case n odd. Analogously, the matrix Q_μ in (3.13) is related to the matrix $G = G_\pm$, defined as follows:

$$[G]_{kj} = \frac{1}{\sqrt{n}} \left(\cos \frac{\pi(2k-1)(2j-1)}{2n} \pm \sin \frac{\pi(2k-1)(2j-1)}{2n} \right),$$

$$k, j = 1, \dots, n, \quad (3.17)$$

by the identity

$$\sqrt{2}G = Q_\mu \begin{pmatrix} \pm I & & \pm J \\ & \pm\sqrt{2} & \\ -J & & I \end{pmatrix}, \quad I = I_{\lfloor n/2 \rfloor}, \quad (3.18)$$

where the central row and column including $\pm\sqrt{2}$ are absent in case n even.

Formulas (3.16) and (3.18) imply that the matrix–vector products $Q_\eta \mathbf{z}$ ($Q_\eta^T \mathbf{z}$) and $Q_\mu \mathbf{z}$ ($Q_\mu^T \mathbf{z}$) can be reduced to matrix–vector products $Q_{\mathcal{H}}^T \mathbf{z}$ ($Q_{\mathcal{H}} \mathbf{z}$) and $G\mathbf{z}$, and vice versa. Notice that the linear transform $Q_{\mathcal{H}} \mathbf{z}$ or $Q_{\mathcal{H}}^T \mathbf{z}$ is the skew-Hartley transform [21], the (-1) -circulant version of the well-known Hartley transform $Q_{\mathcal{H}} \mathbf{z}$. The Hartley and the skew-Hartley transforms are fast transforms (see [8,21] and the references in [8]). We shall see that also the linear transform $G\mathbf{z}$ is fast. These remarks lead to the result stated in the following corollary, regarding the complexity of computations involving matrices from $\mu, \eta, \mathcal{H}, \mathcal{H}$ and from the *new* algebra

$$\gamma = \{Gd(\mathbf{z})G: \mathbf{z} \in \mathbb{C}^n\} \quad (3.19)$$

naturally defined as the set of all matrices diagonalized by the orthonormal matrix $Q_\gamma = G$ in (3.17).

Corollary 3.4. For $\mathcal{L} \in \{\mu, \eta, \mathcal{H}, \mathcal{H}, \gamma\}$, $Q_{\mathcal{L}}$ and $Q_{\mathcal{L}}^T$ define real fast transforms computable in $O(n \log_2 n)$ operations. If $A \in \mathcal{L}$, then $A\mathbf{z}$, for $\mathbf{z} \in \mathbb{C}^n$, can be computed through the transforms $Q_{\mathcal{L}}$ and $Q_{\mathcal{L}}^T$ in the same amount of operations.

Proof. It is enough to show that, for $G^{(n)} = G$, we have

$$G^{(n)} = \frac{1}{\sqrt{2}} E \begin{pmatrix} G^{(n/2)} R_\pm & \mp G^{(n/2)} J R_\mp \\ G^{(n/2)} R_\mp & \pm G^{(n/2)} J R_\pm \end{pmatrix} \quad (n \text{ even}), \quad (3.20)$$

where $R_\pm = D(I \pm J)$, $D = \text{diag}(\cos((2j-1)\pi/(2n)), j = 1, \dots, n/2)$ and E is the permutation matrix $E\mathbf{e}_j = \mathbf{e}_{2j-1}$, $E\mathbf{e}_{n-j+1} = \mathbf{e}_{n-2j+2}$, $j = 1, \dots, n/2$. \square

Notice that, by Proposition 2.4, the algebra γ defined in (3.19) is not a h -space when $n = 2 + 4r$, $r = 0, 1, \dots$. In fact, for these values of n , we have $[G_+]_{2k, r+1} = [G_+]_{2k-1, n-r} = [G_-]_{2k-1, r+1} = [G_-]_{2k, n-r} = 0$, $k = 1, \dots, n/2$. For example, in case $n = 6$,

$$G_+ = \frac{1}{2\sqrt{3}} \begin{pmatrix} \sqrt{3} & 2 & \sqrt{3} & 1 & 0 & -1 \\ 2 & 0 & -2 & 0 & 2 & 0 \\ \sqrt{3} & -2 & \sqrt{3} & -1 & 0 & 1 \\ 1 & 0 & -1 & \sqrt{3} & -2 & \sqrt{3} \\ 0 & 2 & 0 & -2 & 0 & 2 \\ -1 & 0 & 1 & \sqrt{3} & 2 & \sqrt{3} \end{pmatrix} \quad \text{and} \quad G_- = -G_+J.$$

However, by Proposition 2.4, γ is a space of class \mathbb{V} ; in particular, $[G]_{1j} + [G]_{nj} = \pm 2/\sqrt{n} \sin(\pi(2j-1)/2n) \neq 0$, $j = 1, \dots, n$, $\forall n$, and thus γ can be seen, for all n , as the set of all matrices

$$\gamma_{\mathbf{e}_1 + \mathbf{e}_n}(\mathbf{z}) = Gd(G\mathbf{z})d(G(\mathbf{e}_1 + \mathbf{e}_n))^{-1}G, \quad \mathbf{z} \in \mathbb{C}^n. \quad (3.21)$$

In more intuitive terms, the generic matrix of γ is defined by the sum of its first and last row. Thus, by Proposition 2.7, the results in Proposition 2.9 and in Theorem 2.11 can be applied for $\mathcal{L} = \gamma$. For $n \neq 2 + 4r$, γ is also a 1-space because $[G]_{1j} \neq 0 \forall j$. This fact, the equality $T_{0,0}^{-1, -1}G = G \operatorname{diag}(2 \cos((2j-1)\pi/n), j = 1, \dots, n)$ and Theorem 3.1(ii), let us conclude that γ is one of the algebras $\mathcal{C}_-(\cdot; \mathbf{p})$ defined in (3.4) (for $n \neq 2 + 4r$). By using Theorem 3.1 one can find the vector $\tilde{\mathbf{p}} = J\tilde{\mathbf{p}}$ such that $\gamma = \mathcal{C}_-(\cdot; \tilde{\mathbf{p}})$ and then observe that $\mathcal{C}_-(\cdot; \tilde{\mathbf{p}}) = C_{-1}^S + JC_{-1}^{\text{SK}}$. The following proposition shows that the identity $\gamma = C_{-1}^S + JC_{-1}^{\text{SK}}$ holds for all n . This result leads in Corollary 3.7 to an efficient representation, involving the fast transform G , of $(C_{-1} + JC_{-1})_A$ ($A = \text{Hermitian Toeplitz matrix}$).

Proposition 3.5. *If $\gamma = \{Gd(\mathbf{z})G: \mathbf{z} \in \mathbb{C}^n\}$, where G is the orthonormal symmetric and persymmetric matrix in (3.17), then $\gamma = C_{-1}^S + JC_{-1}^{\text{SK}}$.*

Proof. By using (3.18) and the identity $Q_\mu = M_\mu D_\mu$ (M_μ and D_μ are defined in the proof of Theorem 3.3), show that $G = \frac{1}{2}D_\rho F W$, where

$$W = \begin{pmatrix} q_{\pm r_1} & & & & & -\bar{q}_{\pm r_1} \\ & q_{\pm r_2} & & 0 & & -\bar{q}_{\pm r_2} \\ & & \ddots & & & \\ & 0 & & q_{\pm r_{\lfloor n/2 \rfloor}} & & -\bar{q}_{\pm r_{\lfloor n/2 \rfloor}} \\ & & & \pm 2 & & 0 \\ & & \bar{q}_{\pm \bar{r}_{\lfloor n/2 \rfloor}} & & -q_{\pm \bar{r}_{\lfloor n/2 \rfloor}} & \\ & & & & \ddots & \\ \bar{q}_{\pm \bar{r}_2} & & & 0 & & -q_{\pm \bar{r}_2} \\ \bar{q}_{\pm \bar{r}_1} & & & & & -q_{\pm \bar{r}_1} \end{pmatrix},$$

$$q_{\pm} = 1 \pm i, \quad r_j = \rho^{(2j-1)/2}, \quad j = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor$$

(in W the central row and column including ± 2 are absent if n is even). Now let A be a matrix of C_{-1} and denote by D_A the diagonal matrix $(D_{\rho}F)^H A (D_{\rho}F)$. Then

$$GAG = G^H AG = \frac{1}{4} W^H D_A W = \frac{1}{2} (D_A + J D_A J \mp i J D_A \pm i D_A J) \quad (3.22)$$

and, as a consequence,

$$GA^T G = \frac{1}{2} (D_A + J D_A J \mp i D_A J \pm i J D_A). \quad (3.23)$$

For $A = A^T$ (3.22) and (3.23) imply $GAG = \frac{1}{2} (D_A + J D_A J)$. Moreover, for $A^T = -A$, they imply $GJAG = JGAG = \pm \frac{i}{2} (J D_A J - D_A)$. Thus $C_{-1}^S + JC_{-1}^{SK} \subset \gamma$ and the thesis follows because

$$\begin{aligned} \dim(C_{-1}^S + JC_{-1}^{SK}) &= \dim C_{-1}^S + \dim JC_{-1}^{SK} - \dim C_{-1}^S \cap JC_{-1}^{SK} \\ &= \begin{cases} (n+1)/2 + (n-1)/2 - 0 \\ (n/2) + (n/2) - 0 \end{cases} \\ &= n. \quad \square \end{aligned}$$

In the following, the role of C_{β} , τ , \mathcal{H} , \mathcal{K} , η , μ , γ in approximating and in preconditioning Toeplitz matrices is investigated. Let T be an $n \times n$ symmetric Toeplitz matrix, i.e.,

$$T = (t_{|i-j|})_{i,j=1}^n \quad (3.24)$$

for some complex numbers t_0, \dots, t_{n-1} . The well-known optimal preconditioners of T are the best l.s. fits C_T [18], $(C_{-1})_T$ [27], τ_T [6,9,16] and \mathcal{H}_T [8]. (In [31], \mathcal{L}_T is shown to be a good Toeplitz preconditioner also for other seven spaces \mathcal{L} which are all HAs and are associated with fast trigonometric transforms.) As the algebras C and C_{-1} are closed under transposition, by Proposition 2.3, C_T and $(C_{-1})_T$ are symmetric (not only persymmetric) like T . Therefore, $C_T = (C^S)_T$ and $(C_{-1})_T = (C_{-1}^S)_T$, i.e., in order to approximate T , only half of the n parameters defining a circulant or a (-1) -circulant matrix, are exploited. This fact is here a necessary consequence of a general result (Proposition 2.3) and depends, instead of the special form of C or C_{-1} (as, for instance, in [38]), on the more abstract concept of “closure under transposition”. The fact that only half of the n parameters defining a circulant matrix are sufficient for defining C_T is used in [8] to justify the introduction of the Hartley preconditioner \mathcal{H}_T as a fit to T better than the Chan fit C_T . In fact \mathcal{H} , like C , includes C^S , has dimension n and is closed under transposition, but Proposition 2.3 does not imply any a priori restriction on the choice of the parameters defining a \mathcal{H} matrix because matrices from \mathcal{H} are (already) symmetric. For analogous reasons the algebras \mathcal{K} and γ considered in this paper yield fits \mathcal{K}_T and γ_T to T both

better than the Huckle fit $(C_{-1})_T$, and therefore \mathcal{H}_T and γ_T could be new efficient Toeplitz preconditioners, competitive with \mathcal{H}_T . However, while C_T and $(C_{-1})_T$, like T , are simultaneously symmetric and persymmetric, \mathcal{H}_T , \mathcal{K}_T and γ_T are not persymmetric.

Let \mathcal{L} be the $(2n - 2)$ -dimensional space of matrices

$$\tau(\mathbf{z}) + \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \tau(\mathbf{w}) & \vdots \\ 0 & \cdots & 0 \end{pmatrix}, \quad \mathbf{z} \in \mathbb{C}^n, \quad \mathbf{w} \in \mathbb{C}^{n-2}. \quad (3.25)$$

Any matrix of this space is simultaneously symmetric and persymmetric. Moreover, $\mathcal{L}_T = T$ because any symmetric Toeplitz matrix T belongs to \mathcal{L} as is noted in [42] (set $\mathbf{z} = [t_0 t_1 \cdots t_{n-1}]^T$ and $\mathbf{w} = -[t_2 \cdots t_{n-1}]^T$ in (3.25)). Thus, suitable subsets \mathcal{L}' of \mathcal{L} might yield very good fits \mathcal{L}'_T to T , simultaneously symmetric and persymmetric like T . There are at least five matrix algebras simultaneously diagonalized by fast discrete real transforms that are made up with \mathcal{L} matrices. These are τ [2,7,42], τ_{11} and τ_{-1-1} [10,40], and η and μ . They are obtained by setting, respectively, $\mathbf{w} = \mathbf{0}$, $\mathbf{w} = \mp[z_2 \cdots z_{n-1}]$ (see [21]), and $\mathbf{w} = \mp[z_{n-1} \cdots z_2]$ (use (3.7), (3.4)) in (3.25). Problem (2.1) has been solved—in the case $A = T$ —for the algebra τ [6,9,16] and for the algebras τ_{11} and τ_{-1-1} [31] (notice that in [16] problem (2.1) is solved, if $\mathcal{L} = \tau$, for A generic). In this paper, we study η_T and μ_T . As fits to T , they are certainly better than C_T and $(C_{-1})_T$, respectively. Moreover, by the following theorem (Theorem 3.6), they turn out to be also better than \mathcal{H}_T and \mathcal{K}_T or γ_T , respectively.

Theorem 3.6. Assume that $A \in M_n(\mathbb{C})$ is such that $A^T = A = JAJ$. Then

$$\eta_A = (C + JC)_A \quad \text{and} \quad \mu_A = (C_{-1} + JC_{-1})_A. \quad (3.26)$$

As a consequence,

$$\begin{aligned} \|\eta_A - A\|_F &\leq \|\mathcal{L}_A - A\|_F \leq \|C_A - A\|_F \quad \forall \mathcal{L} \in \mathfrak{H}, \\ \|\mu_A - A\|_F &\leq \|\mathcal{L}_A - A\|_F \leq \|(C_{-1})_A - A\|_F \\ &\quad \forall \mathcal{L} \in \mathfrak{K} \text{ and } \mathcal{L} = \gamma. \end{aligned} \quad (3.27)$$

Proof. Let Z_1 and Z_2 be two circulant matrices such that $Z_1 + JZ_2 = (C + JC)_A$. By Proposition 2.3(i), (ii), $Z_1 + JZ_2$ must be simultaneously symmetric and persymmetric like A . This implies $Z_1^T = Z_1$ and $Z_2^T = Z_2$, and therefore $(C + JC)_A \in C^S + JC^S = \eta$. Thus, by the definition of η_A and by the inclusion $\eta \subset C + JC$, $\|\eta_A - A\|_F = \|(C + JC)_A - A\|_F$. Finally, the uniqueness result of Theorem 2.2 yields $\eta_A = (C + JC)_A$. The proof of equality $\mu_A = (C_{-1} + JC_{-1})_A$ is analogous. Inequalities (3.27) follow from the inclusions in Theorem 3.1(iii) and from the fact that $C_A = (C^S)_A$ and $(C_{-1})_A = (C_{-1}^S)_A$ (for the case $\mathcal{L} = \gamma$, $n = 2 + 4r$, use Proposition 3.5). \square

Remark 3. In (3.27), the second inequalities hold also in case A is not persymmetric. The result in (3.27) was first observed for $A = T = (t_{|i-j|})_{i,j=1}^n$, T real, and $n = 3$. In fact, for $p \in \mathbb{R}$, we have $\|\mathcal{C}_+(\cdot; [p-p]^T)_T - T\|_F^2 = \varphi(p)(t_1 - t_2)^2$ and $\|\mathcal{C}_-(\cdot; [p-p]^T)_T - T\|_F^2 = \varphi(p)(t_1 + t_2)^2$, where $\varphi(p) = (10p^2 + 4p + 4)/(9(p^2 + p + 1))$, and one can easily verify that $\varphi(0) < \varphi(p) \forall p \neq 0$. Notice that $\varphi(p) < \varphi(-2) \forall p \neq -2$, and that the algebra $\mathcal{C}_-(\cdot; [-2-2]^T)$ can be shown to coincide with the algebra γ defined in (3.19).

If T is the Toeplitz matrix in (3.24), Theorem 3.6 asserts that η_T (μ_T) is a fit to T better than \mathcal{L}_T for all $\mathcal{L} \in \mathfrak{H} (\mathfrak{K} \cup \{\gamma\})$, and that any \mathcal{L}_T , $\mathcal{L} \in \mathfrak{H} (\mathfrak{K} \cap \{\gamma\})$, is a fit to T better than C_T ($(C_{-1})_T$). It remains to verify if minimizing $\|\mathcal{L}_T - T\|_F$ over $\mathfrak{H} (\mathfrak{K})$ effectively yields more efficient Toeplitz linear systems preconditioners. But first we have to compute η_T and μ_T (see Section 4).

Theorem 3.6 and the linearity of the operator $A \rightarrow \mathcal{L}_A$ (an obvious consequence of the representation of \mathcal{L}_A in Theorem 2.2), let us also find the best l.s. fits from the algebras $C + JC$ and $C_{-1} + JC_{-1}$ to a Hermitian Toeplitz matrix:

Corollary 3.7. *If A is a Hermitian $n \times n$ matrix with persymmetric real part, i.e., $A = X + iY$, where $X, Y \in M_n(\mathbb{R})$, $X^T = X = JXJ$ and $Y^T = -Y$, then*

$$(C + JC)_A = \eta_X + iC_Y \quad \text{and} \quad (C_{-1} + JC_{-1})_A = \mu_X + i(C_{-1})_Y. \quad (3.28)$$

Proof. Set, for instance, $\mathcal{L} = C + JC$. By Theorem 3.6, we have $\mathcal{L}_A = \mathcal{L}_X + i\mathcal{L}_Y = \eta_X + i\mathcal{L}_Y$. Moreover, by Proposition 2.3, \mathcal{L}_Y is skew-symmetric like Y . This implies that \mathcal{L}_Y is circulant, and therefore $\mathcal{L}_Y = C_Y$. \square

A useful representation of the matrix $(C_{-1} + JC_{-1})_A$ in (3.28), involving the fast transform G defined in (3.17), can be obtained as follows. We have $\mu_X + i(C_{-1})_Y = Z_1 + J(Z_2 + iZ_3)$ for some real $Z_1, Z_2 \in C_{-1}^S$ and $Z_3 \in JC_{-1}^{SK}$. As any matrix from C_{-1}^S and JC_{-1}^{SK} is diagonalized by the centrosymmetric matrix $G = Q_\gamma$ in (3.17) (Proposition 3.5), we can write

$$(C_{-1} + JC_{-1})_A = \mu_X + i(C_{-1})_Y = G[D_1 + J(D_2 + iD_3)]G$$

for some real diagonal matrices D_1, D_2, D_3 (for instance, by (3.21), $D_k = d(GZ_k(\mathbf{e}_1 + \mathbf{e}_n))d(G(\mathbf{e}_1 + \mathbf{e}_n))^{-1}$, $k = 1, 2, 3$).

4. Best l.s. fits from η, μ, \mathcal{H} and \mathcal{K}

In this section, an explicit representation (of the first row) of \mathcal{L}_A , $\mathcal{L} \in \{\mu, \eta\}$, where A is an arbitrary $n \times n$ matrix, is obtained. This representation lets us compute \mathcal{L}_A with only $O(n)$ additive operations once that the sums of the entries of each diagonal and of each antidiagonal of A are calculated (see Proposition 4.2). In

particular, we have the result that for a symmetric Toeplitz matrix $T = (t_{|i-j|})_{i,j=1}^n$ the fit \mathcal{L}_T can be computed with the same cost required for the computation of the best-known fits \mathcal{L}_T to T (e.g., C_T , $(C_{-1})_T$, \mathcal{H}_T , τ_T , HAs), i.e., with $O(n)$ arithmetic operations. We also introduce the fit \mathcal{H}_T , the (-1) -circulant version of the fit \mathcal{H}_T defined in [8]. Notice that η_T , μ_T and \mathcal{H}_T have not been previously considered in the literature.

Let $A = (a_{ij})_{i,j=1}^n$ be an arbitrary $n \times n$ matrix with complex entries, and let \mathcal{L}_A be the best l.s. fit to A from $\mathcal{L} \in \{\eta, \mu, \mathcal{H}, \mathcal{H}\}$. Denote by J_s the matrices $\mathcal{L}_1(\mathbf{e}_s)$, $s = 1, \dots, n$, spanning \mathcal{L} . Notice that the J_s are real symmetric matrices (see Theorem 3.1(iv)). By Proposition 2.9 we know that

$$\mathcal{L}_A = \mathcal{L}(B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}) = \sum_{s=1}^n [B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}]_s J_s, \quad (4.1)$$

where $B_{\mathcal{L}}$ is the $n \times n$ positive definite matrix of \mathcal{L}

$$B_{\mathcal{L}} = \sum_{s=1}^n (\text{tr } J_s) J_s, \quad (4.2)$$

and $\mathbf{c}_{\mathcal{L},A}$ is the $n \times 1$ vector

$$[\mathbf{c}_{\mathcal{L},A}]_s = (J_s, A) = \sum_{i,j=1}^n [J_s]_{ij} a_{ij}, \quad s = 1, \dots, n. \quad (4.3)$$

Moreover, by Theorem 3.3, we have

$$\mathcal{L}_A = \mathcal{L}(B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}) = Q_{\mathcal{L}} d(Q_{\mathcal{L}}^T B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}) d(Q_{\mathcal{L}}^T \mathbf{e}_1)^{-1} Q_{\mathcal{L}}^T,$$

where $Q_{\mathcal{L}}$ is the orthonormal matrix defined in (3.10)–(3.13). Therefore, the knowledge of $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}$ is sufficient to obtain a representation of \mathcal{L}_A which is the most useful and convenient in preconditioning techniques. Explicit formulas for the entries of $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}$ are given in Proposition 4.2 in case A is generic and $\mathcal{L} \in \{\eta, \mu\}$, and in Corollaries 4.4 and 4.5 and in Theorem 4.6 in case $A = T$ and $\mathcal{L} \in \{\eta, \mu, \mathcal{H}, \mathcal{H}\}$. A procedure for the computation of $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},T}$, $\mathcal{L} \in \{\eta, \mu\}$, requiring only $O(n)$ arithmetic operations, is suggested by Theorem 4.3. We shall see that the calculus of $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}$ is simplified by the fact that $B_{\mathcal{L}}$ and $B_{\mathcal{L}}^{-1}$ are in \mathcal{L} .

From now on assume that $\mathcal{L} \in \{\mu, \eta\}$. Moreover, in the following, the upper sign refers to the case $\mathcal{L} = \mu$, and the lower sign refers to the case $\mathcal{L} = \eta$. Let us show that

$$B_{\mu} = \begin{cases} n \sum_{k=1}^{n/2} J_{2k-1}, & n \text{ even} \\ \sum_{k=1}^{(n+1)/2} (n+2-2k) J_{2k-1} \\ \quad + \sum_{k=1}^{(n-1)/2} (2k-1) J_{2k}, & n \text{ odd} \end{cases} \quad (J_s = \mu(\mathbf{e}_s)), \quad (4.4)$$

$$B_\eta = \begin{cases} \sum_{k=1}^{n/2} (n - 4k + 4) J_{2k-1}, & n \text{ even} \\ \sum_{k=1}^{(n+1)/2} (n + 2 - 2k) J_{2k-1} & (J_s = \eta(\mathbf{e}_s)). \\ -\sum_{k=1}^{(n-1)/2} (2k - 1) J_{2k}, & n \text{ odd} \end{cases} \quad (4.5)$$

In fact, by formula (4.2), it is enough to calculate $\text{tr } J_s$, $s = 1, \dots, n$. To this aim, use the formulas

$$\text{tr } J_s = \text{tr } \tau(\mathbf{e}_s) \pm \text{tr } \tau(\mathbf{e}_{n-s}^{(n-2)}) \quad \left(\text{tr } \tau(\mathbf{e}_s) = \begin{cases} n - s + 1, & s \text{ odd} \\ 0, & s \text{ even} \end{cases} \right),$$

where $\mathbf{e}_k^{(n-2)}$ is the $(n-2) \times 1$ vector $[0 \ \dots \ 0 \ \overset{k}{1} \ 0 \ \dots \ 0]^T$, which follow from (3.4) and (3.7).

Notice that, once expressions (4.4) and (4.5) for $B_{\mathcal{L}}$ are available, the inverse $B_{\mathcal{L}}^{-1}$ can be obtained, at least from an heuristic point of view, by looking for vectors \mathbf{z} such that $\mathbf{z}^T B_{\mathcal{L}} = \mathbf{e}_1^T$ or, equivalently, such that $\mathcal{L}(\mathbf{z}) B_{\mathcal{L}} = I$ (see Proposition 2.6(iv)):

$$B_\mu^{-1} = \begin{cases} \frac{1}{2n}(3J_1 - J_{n-1}), & n \text{ even} \\ \frac{1}{2n}(3J_1 - J_{n-1}) & (J_s = \mu(\mathbf{e}_s)), \\ -\frac{1}{n^2} \sum_{i=1}^n (-1)^{i-1} J_i, & n \text{ odd} \end{cases} \quad (4.6)$$

$$B_\eta^{-1} = \begin{cases} \frac{1}{2n}(3J_1 + J_{n-1}) - \frac{2}{n^2} \sum_{k=1}^{n/2} J_{2k-1}, & n \text{ even} \\ \frac{1}{2n}(3J_1 + J_{n-1}) - \frac{1}{n^2} \sum_{i=1}^n J_i, & n \text{ odd} \end{cases} \quad (J_s = \eta(\mathbf{e}_s)). \quad (4.7)$$

We give a direct proof only of (4.6) for n even. In the other cases, we simply display $E = B_{\mathcal{L}}^{-1}$ in (4.10) and (4.11).

Assume $\mathcal{L} = \mu$. Let n be even, and set $E = \frac{1}{2n}(3J_1 - J_{n-1})$. By exploiting Proposition 3.2, case μ , one can write down the μ matrix E :

$$E = \frac{1}{2n} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 3 & & & -1 & 0 \\ 2 & & \mathbf{0} & -1 & 0 & -1 \\ & \ddots & & & & -1 \\ & & 2 & -1 & \ddots & \ddots \\ & & & 1 & 0 & -1 \\ \mathbf{0} & & & & & \mathbf{0} \\ & & -1 & 0 & 1 & \\ & \ddots & -1 & & 2 & \\ & -1 & \ddots & \ddots & & \ddots \\ -1 & 0 & -1 & & & 2 \\ 0 & -1 & & \mathbf{0} & & 3 \end{pmatrix}. \quad (4.8)$$

Notice that

$$\begin{aligned}
\mathbf{e}_1^T E &= \frac{1}{2n}(3\mathbf{e}_1 - \mathbf{e}_{n-1})^T, \\
\mathbf{e}_s^T E &= \frac{1}{2n}(2\mathbf{e}_s - \mathbf{e}_{n-s} - \mathbf{e}_{n-s+2})^T, \quad s = 2, \dots, n-1, \\
\mathbf{e}_n^T E &= \frac{1}{2n}(3\mathbf{e}_n - \mathbf{e}_2)^T.
\end{aligned} \tag{4.9}$$

Therefore, by (4.4),

$$\begin{aligned}
\mathbf{e}_1^T B_\mu E &= n \left(\sum_{k=1}^{n/2} \mathbf{e}_{2k-1}^T \right) E \\
&= n \left(\mathbf{e}_1^T E + \sum_{k=2}^{n/2} \mathbf{e}_{2k-1}^T E \right) \\
&= \frac{1}{2} \left[3\mathbf{e}_1 - \mathbf{e}_{n-1} + \sum_{k=2}^{n/2} (2\mathbf{e}_{2k-1} - \mathbf{e}_{n-2k+1} - \mathbf{e}_{n-2k+3}) \right]^T \\
&= \mathbf{e}_1^T,
\end{aligned}$$

i.e., the first row of $B_\mu E$ is equal to the first row of the identity matrix I . Then $B_\mu E = I$, because $B_\mu E, I \in \mu$.

For $\mathcal{L} = \eta$, n even, we obtain:

$$E = \frac{1}{2n} \begin{pmatrix} 1 & 0 & & \dots & & 0 & 0 \\ & 2 & & & \mathbf{0} & & 1 & 0 & 1 \\ & & \ddots & & & & \ddots & \ddots & 1 \\ & & & 2 & & 1 & \ddots & \ddots & \\ & & & & 3 & 0 & 1 & \ddots & \\ \mathbf{0} & & & & & & & & \mathbf{0} \\ & & & 1 & 0 & 3 & & & \\ & & \ddots & \ddots & 1 & & 2 & & \\ & 1 & \ddots & \ddots & & \mathbf{0} & & \ddots & \\ 1 & 0 & 1 & & & & & 2 & \\ 0 & 1 & & & & & & & 3 \end{pmatrix} - \frac{2}{n^2}(\mathbf{a}\mathbf{a}^T + \mathbf{b}\mathbf{b}^T), \tag{4.10}$$

$$\mathbf{a} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 1 \end{bmatrix}.$$

Finally, for $\mathcal{L} \in \{\mu, \eta\}$, n odd, we have

$$E = \frac{1}{2n} \begin{pmatrix} & 1 & 0 & \cdots & 0 & 0 \\ & 2 & & \mathbf{0} & \mp 1 & 0 & \mp 1 \\ & & \ddots & & \mp 1 & 0 & \mp 1 \\ & & & 2 & \mp 1 & 0 & \\ \mathbf{0} & & & \mp 1 & 2 & \mp 1 & \mathbf{0} \\ & & \ddots & 0 & \mp 1 & 2 & \\ & \mp 1 & & \ddots & & \ddots & \\ \mp 1 & 0 & \mp 1 & & \mathbf{0} & & 2 \\ 0 & \mp 1 & & & & & 3 \end{pmatrix} - \frac{1}{n^2} \mathbf{a} \mathbf{a}^T, \quad (4.11)$$

$$\mathbf{a} = \begin{bmatrix} 1 \\ \mp 1 \\ 1 \\ \mp 1 \\ \vdots \\ 1 \\ \mp 1 \\ 1 \end{bmatrix}.$$

By using formulas (4.9)–(4.11) one can state a set of identities connecting the rows $i - 1$ with $i + 1$ and k with $n + 2 - k$ of $B_{\mathcal{L}}^{-1}$, $\mathcal{L} \in \{\mu, \eta\}$. These identities can be immediately translated (use (4.3)) into relations among the entries of the vector $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L}, A}$ defining \mathcal{L}_A . Set $\psi^{\mathcal{L}, A} = B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L}, A}$.

Lemma 4.1. *If A is an arbitrary $n \times n$ matrix and $\mathcal{L} \in \{\eta, \mu\}$, then*

$$\psi_{i+1}^{\mathcal{L}, A} = \psi_{i-1}^{\mathcal{L}, A} + \frac{1}{2n} \times \begin{cases} (2J_3 - 2J_1 \mp J_{n-3} - J_1, A), & i = 2, \\ (2J_{i+1} - 2J_{i-1} \pm J_{n-i+3} \mp J_{n-i-1}, A), & i = 3, \dots, n-2, \\ (2J_n - 2J_{n-2} \pm J_4 + J_n, A), & i = n-1, \end{cases} \quad (4.12)$$

and

$$\psi_{n+2-k}^{\mathcal{L},A} = \mp \psi_k^{\mathcal{L},A} + \frac{1}{2n} \times \begin{cases} (\pm J_2 + 2J_n - J_{n-2}, A), & k = 2, \\ (\pm J_k + J_{n-k+2} - J_{n-k} \mp J_{k-2}, A), & k = 3, \dots, n-1. \end{cases} \quad (4.13)$$

We shall see that Lemma 4.1 suggests a simple procedure for an explicit and numerical computation of the vector $\psi^{\mathcal{L},A}$ when A is a symmetric Toeplitz matrix T .

In the following proposition, the entries of $\psi^{\mathcal{L},A}$, A generic, are represented via simple formulas in terms of the scalars

$$\begin{aligned} d_1^\lambda &= \sum_{j=1}^n a_{jj}, \\ d_k^\lambda &= \sum_{j=1}^{n-k+1} (a_{j,k+j-1} + a_{k+j-1,j}), \quad k = 2, \dots, n, \\ d_n' &= \sum_{j=1}^n a_{j,n+1-j}, \\ d_k' &= \sum_{j=1}^k (a_{j,k+1-j} + a_{n-k+j,n-j+1}), \quad k = n-1, \dots, 1. \end{aligned} \quad (4.14)$$

Proposition 4.2. Let $A = (a_{ij})_{i,j=1}^n$ be an arbitrary $n \times n$ matrix and let $\mathcal{L}_A = \mathcal{L}(\psi^{\mathcal{L},A})$ be the best l.s. fit to A from $\mathcal{L} \in \{\eta, \mu\}$. Then for n even

$$\psi_s^{\mu,A} = \frac{1}{2n} \times \begin{cases} (2d_1^\lambda + d_1' - d_{n-1}'), & s = 1, \\ (d_s^\lambda - d_{n-s+2}^\lambda + d_s' - d_{n-s}'), & s = 2, \dots, n-1, \\ (d_n^\lambda - d_2^\lambda + 2d_n'), & s = n, \end{cases} \quad (4.15)$$

$$\psi_s^{\eta,A} = \frac{1}{2n} \times \begin{cases} (2d_1^\lambda + d_1' + d_{n-1}') - (4/n)f, & s = 1, \\ (d_s^\lambda + d_{n-s+2}^\lambda + d_s' + d_{n-s}') - \frac{4}{n} \times \begin{cases} (g) & s \text{ even}, \\ (f) & s \text{ odd}, \end{cases} & s = 2, \dots, n-1, \\ (d_n^\lambda + d_2^\lambda + 2d_n') - (4/n)g, & s = n, \end{cases} \quad (4.16)$$

and, for n odd,

$$\psi_s^{\mathcal{L},A} = \frac{1}{2n} \times \begin{cases} (2d_1^{\setminus} + d_1^{\setminus} \mp d_{n-1}^{\setminus}) \\ \quad -(2/n)(f \mp g), & s = 1, \\ (d_s^{\setminus} \mp d_{n-s+2}^{\setminus} + d_s^{\setminus} \mp d_{n-s}^{\setminus}) \\ \quad -(2/n)(\mp 1)^{s-1}(f \mp g), & s = 2, \dots, n-1, \\ (d_n^{\setminus} \mp d_2^{\setminus} + 2d_n^{\setminus}) \\ \quad -(2/n)(f \mp g), & s = n, \end{cases} \quad (4.17)$$

where $f = \sum_{k=1}^{\lceil n/2 \rceil} d_{2k-1}^{\setminus}$ and $g = \sum_{k=1}^{\lfloor n/2 \rfloor} d_{2k}^{\setminus}$. Thus, if the d_k^{\setminus} , d_k^{\setminus} in (4.14) are given, then the vector $2n\psi^{\mathcal{L},A}$ can be computed in $O(n)$ additive operations.

Proof. Formulas (4.15)–(4.17) are easily obtained from the identities

$$\psi_s^{\mathcal{L},A} = \sum_{k=1}^n [B_{\mathcal{L}}^{-1}]_{sk}(J_k, A) = (\mathcal{L}(B_{\mathcal{L}}^{-1}\mathbf{e}_s), A), \quad s = 1, \dots, n,$$

by displaying the matrices $\mathcal{L}(B_{\mathcal{L}}^{-1}\mathbf{e}_s)$ and by expressing each of them as the sum of a matrix from $C_{\mp 1}^S$ and of a matrix from $JC_{\mp 1}^S$. \square

By Proposition 4.2 the total amount of computation required to calculate the vector $2n\psi^{\mathcal{L},A}$ is $O(n^2)$ additive operations (no significant multiplication is required). Obviously, the cost of the computation of the scalars in (4.14) reduces by a factor $\frac{1}{2}$ if $A^T = A$ (or if $A^T = JAJ$), and by a factor $\frac{1}{4}$ if $A^T = A = JAJ$. Notice that if A is simultaneously symmetric and persymmetric, the matrices η_A and μ_A are good approximations of A , because, by Theorem 3.6, $\eta_A = (C + JC)_A$ and $\mu_A = (C_{-1} + JC_{-1})_A$. Thus, the formulas in Proposition 4.2 could be useful even if A is not Toeplitz.

Now choose $A = T = (t_{|i-j|})_{i,j=1}^n$ and set $s_i^{\pm} = t_i \pm t_{n-i}$, $i = 1, \dots, n-1$. Observe that $s_i^{\pm} = \pm s_{n-i}^{\pm}$. By using the fact that the matrices $\pm J_2 + 2J_n - J_{n-2}$ and $\pm J_k + J_{n-k+2} - J_{n-k} \mp J_{k-2}$, $k = 3, \dots, \lceil (n+1)/2 \rceil$, are in $JC_{\mp 1}^S$ and the fact that the matrices $J_k \mp J_{n+2-k}$, $k = 2, \dots, \lceil (n+1)/2 \rceil$, are in $C_{\mp 1}^S$, we obtain

$$\begin{aligned} (\pm J_2 + 2J_n - J_{n-2}, T) &= \pm 4s_1^{\pm}, \\ (\pm J_k + J_{n-k+2} - J_{n-k} \mp J_{k-2}, T) &= \pm 4s_{k-1}^{\pm}, \quad k = 3, \dots, n-1, \\ (J_1, T) &= nt_0, \\ (J_k \mp J_{n+2-k}, T) &= 2nt_{k-1} - 2(k-1)s_{k-1}^{\pm}, \quad k = 2, \dots, n. \end{aligned} \quad (4.18)$$

These formulas and the identities

$$\begin{aligned} (2J_3 - 2J_1 \mp J_{n-3} - J_1, T) \\ = (\pm J_{n-1} + J_3 - J_1 \mp J_{n-3}, T) + (J_3 \mp J_{n-1}, T) - 2(J_1, T), \end{aligned}$$

$$\begin{aligned}
& (2J_{i+1} - 2J_{i-1} \pm J_{n-i+3} \mp J_{n-i-1}, T) \\
& = (\pm J_{n-i+1} + J_{i+1} - J_{i-1} \mp J_{n-i-1}, T) \\
& \quad + (J_{i+1} \mp J_{n-i+1}, T) - (J_{i-1} \mp J_{n-i+3}, T), \quad i = 3, \dots, n-2, \\
& (2J_n - 2J_{n-2} \pm J_4 + J_n, T) \\
& = (\pm J_2 + 2J_n - J_{n-2}, T) + (J_n \mp J_2, T) - (J_{n-2} \mp J_4, T)
\end{aligned} \tag{4.19}$$

let us rewrite (4.12) and (4.13) as in Theorem 4.3. Theorem 4.3 also includes the specifications of some of formulas (4.15)–(4.17) for the case $A = T$. In the following, $\delta_{s,o}$ is 1 (0) if s is odd (even), and $\delta_{s,e}$ is 1 (0) if s is even (odd).

Theorem 4.3. Let $T = (t_{|i-j|})_{i,j=1}^n$ and $\mathcal{L} \in \{\eta, \mu\}$. Then

$$\psi_{i+1}^{\mathcal{L},T} = \psi_{i-1}^{\mathcal{L},T} + t_i - t_{i-2} + \frac{i-2}{n}(s_{i-2}^{\pm} - s_i^{\pm}), \quad i = 2, \dots, n-1, \tag{4.20}$$

$$\psi_{n+2-i}^{\mathcal{L},T} = \mp \psi_i^{\mathcal{L},T} \pm \frac{2}{n}s_{i-1}^{\pm}, \quad i = 2, \dots, n, \tag{4.21}$$

where

$$s_i^{\pm} = t_i \pm t_{n-i}, \quad i = 0, \dots, n \quad (t_n = \mp t_0), \tag{4.22}$$

and the following initial conditions hold:

$$n \text{ even} \quad \begin{cases} \psi_1^{\mu,T} = t_0 - \frac{2}{n} \left(\sum_{j=1}^{\lceil n/4 \rceil - 1} s_{2j}^+ + t_{n/2} \delta_{n/2,e} \right), \\ \psi_n^{\mu,T} = t_{n-1} - \frac{n-1}{n} s_{n-1}^+ + \frac{2}{n} \left(\sum_{j=1}^{\lfloor n/4 \rfloor} s_{2j-1}^+ + t_{n/2} \delta_{n/2,o} \right), \end{cases} \tag{4.23}$$

$$n \text{ even} \quad \begin{cases} \psi_1^{\eta,T} = t_0 + \frac{4}{n^2} \left(\sum_{j=1}^{\lceil n/4 \rceil - 1} 2js_{2j}^- - \frac{n}{2} \sum_{j=1}^{\lceil n/4 \rceil - 1} s_{2j}^- \right), \\ \psi_n^{\eta,T} = t_{n-1} - \frac{n-1}{n} s_{n-1}^- \\ \quad + \frac{4}{n^2} \left[\sum_{j=1}^{\lfloor n/4 \rfloor} (2j-1)s_{2j-1}^- - \frac{n}{2} \sum_{j=1}^{\lfloor n/4 \rfloor} s_{2j-1}^- \right], \end{cases} \tag{4.24}$$

$$n \text{ odd} \quad \begin{cases} \psi_1^{\mathcal{L},T} = t_0 \mp \frac{2}{n^2} \left(\sum_{j=1}^{(n-1)/2} (\mp 1)^{j-1} js_j^{\pm} \pm n \sum_{j=1}^{\lfloor (n-1)/4 \rfloor} s_{2j}^{\pm} \right), \\ \psi_n^{\mathcal{L},T} = t_{n-1} - \frac{n-1}{n} s_{n-1}^{\pm} \\ \quad \mp \frac{2}{n^2} \left(\sum_{j=1}^{(n-1)/2} (\mp 1)^{j-1} js_j^{\pm} - n \sum_{j=1}^{\lfloor (n+1)/4 \rfloor} s_{2j-1}^{\pm} \right). \end{cases} \tag{4.25}$$

Proof. Formulas for $\psi_1^{\mathcal{L},T}$ and $\psi_n^{\mathcal{L},T}$ in terms of the scalars t_0, t_1, \dots, t_{n-1} , can be easily obtained by using the identities $\psi_1^{\mathcal{L},T} = (B_{\mathcal{L}}^{-1}, T)$ and $\psi_n^{\mathcal{L},T} = (JB_{\mathcal{L}}^{-1}, T)$, and expressions (4.8), (4.10) and (4.11) of $B_{\mathcal{L}}^{-1}$. (Consider separately the contribution of the terms $\frac{1}{2n}(2I) \left(\frac{1}{2n}(2J) \right)$ in the expressions of $B_{\mathcal{L}}^{-1} (JB_{\mathcal{L}}^{-1})$.) These formulas can be rewritten as in (4.23)–(4.25) by using the notation in (4.22). \square

Theorem 4.3 suggests a simple procedure for the computation of $\psi^{\mathcal{L},T}$, which requires only $O(n)$ arithmetic operations: calculate $\psi_i^{\mathcal{L},T}$, $i = 1, n$, by (4.23)–(4.25) (for n odd $\psi_1^{\mathcal{L},T}$ would be enough) and then calculate all other entries $\psi_i^{\mathcal{L},T}$ by (4.20) and (4.21). Moreover, Theorem 4.3 and inductive arguments let us calculate each entry of $\psi^{\mathcal{L},T}$ explicitly as in the following corollaries [Corollaries 4.4 (μ_T) and 4.5 (η_T)]. These results are exploited, respectively, in the following section and in Proposition 4.7, to show that the best l.s. fits η_T and μ_T satisfy a standard “clustering” property of Toeplitz preconditioners, and to calculate the eigenvalues of η_T and μ_T . The same results will be exploited in Theorem 6.1 to find explicit formulas of the “errors” $\|\eta_T - T\|_F$ and $\|\mu_T - T\|_F$.

Corollary 4.4 (μ_T). *We have*

$$\psi_i^{\mu,T} = [B_\mu^{-1} \mathbf{c}_{\mu,T}]_i = a_{i-1} + b_{n-i}, \quad i = 1, \dots, n, \quad (4.26)$$

where

$$\begin{aligned} a_j &= t_j - \frac{j}{n} s_j^+, \quad j = 0, \dots, n-1 \\ (a_{n-j} &= -a_j, \quad j = 1, \dots, n-1), \end{aligned} \quad (4.27)$$

and, for n even,

$$\begin{aligned} b_{2k} &= \frac{2}{n} \left(\sum_{j=k+1}^{\lfloor n/4 \rfloor} s_{2j-1}^+ + t_{n/2} \delta_{n/2,o} \right), \quad k = 0, 1, \dots, \lfloor n/4 \rfloor, \\ b_{2k-1} &= \frac{2}{n} \left(\sum_{j=k}^{\lfloor n/4 \rfloor - 1} s_{2j}^+ + t_{n/2} \delta_{n/2,e} \right), \quad k = 1, \dots, \lfloor n/4 \rfloor, \\ b_{n-j} &= -b_j, \quad j = 1, \dots, n/2 - 1, n/2, \end{aligned} \quad (4.28)$$

and, for n odd,

$$\begin{aligned} b_{2k} &= -\frac{2}{n^2} \left[\sum_{j=1}^{(n-1)/2} (-1)^{j-1} j s_j^+ - n \sum_{j=k+1}^{\lfloor (n+1)/4 \rfloor} s_{2j-1}^+ \right], \\ k &= 0, 1, \dots, \lfloor (n+1)/4 \rfloor, \\ b_{2k-1} &= \frac{2}{n^2} \left[\sum_{j=1}^{(n-1)/2} (-1)^{j-1} j s_j^+ + n \sum_{j=k}^{\lfloor (n-1)/4 \rfloor} s_{2j}^+ \right], \\ k &= 1, \dots, \lfloor (n-1)/4 \rfloor + 1, \\ b_{n-j} &= -b_j, \quad j = 1, \dots, (n-1)/2. \end{aligned} \quad (4.29)$$

Thus, $\mu_T = (C_{-1})_T + JR_{\mu,T}$, where $(C_{-1})_T, R_{\mu,T} \in C_{-1}^S$ and $[(C_{-1})_T]_{1j} = a_{j-1}$, $[R_{\mu,T}]_{1j} = b_{j-1}$, $j = 1, \dots, n$.

Corollary 4.5 (η_T). *We have*

$$\psi_i^{\eta,T} = [B_\eta^{-1} \mathbf{c}_{\eta,T}]_i = a_{i-1} + b_{n-i}, \quad i = 1, \dots, n, \quad (4.30)$$

where

$$\begin{aligned} a_j &= t_j - \frac{j}{n} s_j^-, \quad j = 0, \dots, n-1 \\ (a_{n-j} &= a_j, \quad j = 1, \dots, n-1), \end{aligned} \quad (4.31)$$

and, for n even,

$$\begin{aligned} b_{2k} &= \frac{4}{n^2} \left[\sum_{j=1}^{\lfloor n/4 \rfloor} (2j-1) s_{2j-1}^- - \frac{n}{2} \sum_{j=k+1}^{\lfloor n/4 \rfloor} s_{2j-1}^- \right], \\ k &= 0, 1, \dots, \lfloor n/4 \rfloor, \\ b_{2k-1} &= \frac{4}{n^2} \left(\sum_{j=1}^{\lfloor n/4 \rfloor - 1} 2j s_{2j}^- - \frac{n}{2} \sum_{j=k}^{\lfloor n/4 \rfloor - 1} s_{2j}^- \right), \\ k &= 1, \dots, \lfloor n/4 \rfloor, \\ b_{n-j} &= b_j, \quad j = 1, \dots, n/2 - 1, n/2, \end{aligned} \quad (4.32)$$

and, for n odd,

$$\begin{aligned} b_{2k} &= \frac{2}{n^2} \left(\sum_{j=1}^{(n-1)/2} j s_j^- - n \sum_{j=k+1}^{\lfloor (n+1)/4 \rfloor} s_{2j-1}^- \right), \\ k &= 0, 1, \dots, \lfloor (n+1)/4 \rfloor, \\ b_{2k-1} &= \frac{2}{n^2} \left(\sum_{j=1}^{(n-1)/2} j s_j^- - n \sum_{j=k}^{\lfloor (n-1)/4 \rfloor} s_{2j}^- \right), \\ k &= 1, \dots, \lfloor (n-1)/4 \rfloor + 1, \\ b_{n-j} &= b_j, \quad j = 1, \dots, (n-1)/2. \end{aligned} \quad (4.33)$$

Thus, $\eta_T = C_T + JR_{\eta,T}$, where $C_T, R_{\eta,T} \in C^S$ and $[C_T]_{1j} = a_{j-1}$, $[R_{\eta,T}]_{1j} = b_{j-1}$, $j = 1, \dots, n$.

The main steps of the proofs of both Corollaries 4.4 and 4.5 are the following: for n even and $\mathcal{L} = \mu(\eta)$ prove inductively equality (4.26) (Eq. (4.30)), respectively, for $i = 1, 3, \dots, 2\lfloor n/4 \rfloor - 1$; for $i = n, n-2, \dots, n-2\lfloor (n-2)/4 \rfloor$; for

$i = 2, 4, \dots, 2\lfloor n/4 \rfloor$; for $i = n - 1, n - 3, \dots, n - 2\lfloor n/4 \rfloor + 1$, by using formulas (4.23) ((4.24)), (4.20) and (4.21). The case n odd is similar.

Remark 4. In Corollary 4.4 (μ_T), case n even, one observes that the entries $\psi_i^{\mu,T}$ simplify when i approaches the value $\frac{n}{2} + 1$. In particular, $\psi_{n/2}^{\mu,T} = t_{n/2-1} - ((n/2 - 1)/n)s_{n/2-1}^+$, $\psi_{n/2+1}^{\mu,T} = \frac{1}{n}s_{n/2}^+$ and $\psi_{n/2+2}^{\mu,T} = t_{n/2+1} - ((n/2 - 1)/n)s_{n/2-1}^+$. Therefore, to compute $\psi_i^{\mu,T}$ as suggested by Theorem 4.3, it is convenient to use as initial values in (4.20), (4.21), $\psi_{n/2}$ and $\psi_{n/2+1}$ or $\psi_{n/2+1}$ and $\psi_{n/2+2}$ instead of ψ_1 and ψ_n . For analogous but less clear reasons, this is also true for n odd (use $\psi_{(n+1)/2}$ or $\psi_{(n+3)/2}$ instead of ψ_1) and in the η case.

The results of Theorem 4.3 or Corollaries 4.4 and 4.5 can also be used to calculate the best l.s. fits from $\mathcal{L} = \eta, \mu$, to a matrix A that is equal to a centrosymmetric Toeplitz plus Hankel matrix but a low-rank perturbation in at most $O(n \log_2 n)$ arithmetic operations. In fact the vector $B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},A}$ can be computed by applying Theorem 4.3 twice and then by performing a low number of fast transforms. This remark is an obvious consequence of the equalities

$$B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},M'+MJ} = B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},M'} + J B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},M} \quad (4.34)$$

and

$$B_{\mathcal{L}}^{-1} \mathbf{c}_{\mathcal{L},\mathbf{xy}^T} = B_{\mathcal{L}}^{-1} \mathcal{L}(\mathbf{x})\mathbf{y} \quad (4.35)$$

which hold for arbitrary $n \times n$ matrices M and M' and vectors $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. In order to prove (4.34) simply observe that $\mathbf{c}_{\mathcal{L},MJ} = J \mathbf{c}_{\mathcal{L},M}$, in fact $[\mathbf{c}_{\mathcal{L},MJ}]_k = (J_k, MJ) = (J_k J, M) = (J_{n+1-k}, M) = [\mathbf{c}_{\mathcal{L},M}]_{n+1-k}$. Regarding (4.35) it is sufficient to calculate (see Proposition 2.6(v)) $[\mathbf{c}_{\mathcal{L},\mathbf{xy}^T}]_k = (J_k, \mathbf{xy}^T) = \mathbf{x}^T J_k \mathbf{y} = [\mathcal{L}(\mathbf{x})\mathbf{y}]_k$. Notice how these results depend on the fact that J and $B_{\mathcal{L}}^{-1}$ belong to \mathcal{L} .

In the following theorem, we obtain the fit \mathcal{H}_T . We also list, in Proposition 4.7, the eigenvalues of \mathcal{L}_T , $\mathcal{L} \in \{\mu, \eta, \mathcal{H}, \mathcal{H}\}$, which are calculated by using equality (3.9) in Theorem 3.3.

Theorem 4.6. Let $\mathcal{H}_T = \mathcal{H}(B_{\mathcal{H}}^{-1} \mathbf{c}_{\mathcal{H},T})$ ($\mathcal{H}_T = \mathcal{H}(B_{\mathcal{H}}^{-1} \mathbf{c}_{\mathcal{H},T})$) be the best l.s. fit to T from the algebra $\mathcal{H}(\mathcal{H})$. Then

$$[B_{\mathcal{H}}^{-1} \mathbf{c}_{\mathcal{H},T}]_i = \frac{1}{n} [\mathbf{c}_{\mathcal{H},T}]_i = a_{i-1} - b_{i-1}$$

$$\left([B_{\mathcal{H}}^{-1} \mathbf{c}_{\mathcal{H},T}]_i = \frac{1}{n} [\mathbf{c}_{\mathcal{H},T}]_i = a_{i-1} + b_{i-1} \right), \quad i = 1, \dots, n,$$

where $a_j = t_j - \frac{j}{n}s_j^+$ ($a_j = t_j - \frac{j}{n}s_j^-$), $j = 0, \dots, n-1$, and $b_j = -s_j^+/n$ ($b_j = s_j^-/n$), $j = 0, \dots, n-1$. Thus, $\mathcal{H}_T = (C_{-1})_T + J P_{-1} R_{\mathcal{H},T}$ ($\mathcal{H}_T = C_T + J P R_{\mathcal{H},T}$), where $R_{\mathcal{H},T}$ ($R_{\mathcal{H},T}$) is the skewsymmetric (-1)-circulant (circulant) matrix with first row $[b_0 \ b_1 \ \dots \ b_{n-1}]$.

Proposition 4.7. Let $T = (t_{|i-j|})_{i,j=1}^n$, $t_k \in \mathbb{C}$. Then the eigenvalues of μ_T , η_T , \mathcal{K}_T and \mathcal{H}_T are, respectively,

$$\begin{aligned} z_{-,j} \pm \frac{1}{\sin \alpha_{-,j}} w_{-,j}, \quad j = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor, \quad z_{-, (n+1)/2} \quad (n \text{ odd}), \\ z_{+,1}, z_{+,j} \mp \frac{1}{\sin \alpha_{+,j}} w_{+,j}, \quad j = 2, \dots, \left\lceil \frac{n}{2} \right\rceil, \quad z_{+, \frac{n}{2}+1} \quad (n \text{ even}), \\ z_{-,j} + w_{-,j}, \quad j = 1, \dots, n, \\ z_{+,j} + w_{+,j}, \quad j = 1, \dots, n, \end{aligned}$$

where, for $j = 1, \dots, n$,

$$\begin{aligned} \alpha_{-,j} &= \frac{\pi(2j-1)}{n}, \quad \alpha_{+,j} = \frac{2\pi(j-1)}{n}, \\ z_{\mp,j} &= t_0 + 2 \sum_{r=1}^{n-1} t_r \cos(r\alpha_{\mp,j}) - \frac{2}{n} \sum_{r=1}^{n-1} r t_r \cos(r\alpha_{\mp,j}), \\ w_{\mp,j} &= \frac{2}{n} \sum_{r=1}^{n-1} t_r \sin(r\alpha_{\mp,j}). \end{aligned}$$

In the following section, μ_A , η_A and \mathcal{K}_A will be studied as preconditioners in the CG algorithm for solving positive definite linear systems. In [22], it is shown that the same matrices can also be exploited in quasi-Newtonian iterative schemes for minimum problems.

5. Best l.s. fits as preconditioners of positive definite systems

The aim of this section is to show that the fits \mathcal{L}_T , $\mathcal{L} \in \{\eta, \mu, \mathcal{K}\}$, satisfy all properties that a good Toeplitz linear system preconditioner should have. These properties are first investigated for generic positive definite linear systems. In the following all matrices, vectors and scalars are real. Moreover, for a positive definite matrix A , $\lambda_1(A)$, $\lambda_2(A)$, \dots , $\lambda_n(A)$ denote the eigenvalues of A in nondecreasing order; $c(A)$ denotes the spectral condition number of A , $c(A) = \lambda_n(A)/\lambda_1(A)$; and $\|\cdot\|_A$ denotes the energy norm corresponding to A , $\|\mathbf{z}\|_A = \sqrt{\mathbf{z}^T A \mathbf{z}}$, $\mathbf{z} \in \mathbb{R}^n$.

Let $A^{(n)}$, $n = 1, 2, \dots$, be a sequence of positive definite $n \times n$ matrices and assume that there exist $a_{\min} < a_{\max}$ such that

$$0 < a_{\min} \leq \lambda_i(A^{(n)}) \leq a_{\max} \quad \forall i, n, \quad (5.1)$$

and thus $c(A^{(n)}) = \lambda_n(A^{(n)})/\lambda_1(A^{(n)}) \leq M \equiv a_{\max}/a_{\min} \quad \forall n$. Observe that, if $\{A^{(n)}\}_{n=1}^{+\infty}$ is a “nested” sequence, i.e., $A^{(n)}$ is the $n \times n$ upper-left submatrix of $A^{(n+1)}$, then (5.1) is equivalent to the requirement that the condition numbers of the

$A^{(n)}$ are uniformly bounded because, in that case, the eigenvalues of $A^{(n)}$ separate those of $A^{(n+1)}$. For an arbitrarily fixed n consider the linear system

$$A^{(n)}\mathbf{x} = \mathbf{b}^{(n)}, \quad \mathbf{b}^{(n)} \in \mathbb{R}^n. \quad (5.2)$$

System (5.2) has a unique solution, $\mathbf{x}^{(n)} = A^{(n)-1}\mathbf{b}^{(n)}$, and the CG method can be efficiently applied to solve it. In fact, the CG method yields, in principle, an approximation of $\mathbf{x}^{(n)}$ of arbitrary accuracy in only $O(\Phi(A^{(n)}\mathbf{f}^{(n)}))$ arithmetic operations, where $\Phi(A^{(n)}\mathbf{f}^{(n)})$ is the number of arithmetic operations required to perform the matrix–vector product $A^{(n)}\mathbf{f}^{(n)}$, $\mathbf{f}^{(n)} \in \mathbb{R}^n$, the most expensive operation at each step of the method. More specifically, if $\mathbf{x}_q^{(n)}$ is the approximation of $\mathbf{x}^{(n)}$ obtained after q steps of the CG method, and $\sigma_q^{(n)} = \|\mathbf{x}_q^{(n)} - \mathbf{x}^{(n)}\|_{A^{(n)}}$, then

$$\frac{\sigma_q^{(n)}}{\sigma_0^{(n)}} \leq 2 \left(\frac{\sqrt{c(A^{(n)})} - 1}{\sqrt{c(A^{(n)})} + 1} \right)^q \leq u_q = 2 \left(\frac{\sqrt{M} - 1}{\sqrt{M} + 1} \right)^q \quad \forall \mathbf{x}_0^{(n)} \in \mathbb{R}^n \quad (5.3)$$

(see [1] for the first inequality), and thus for any fixed $\delta > 0$, the least number q of steps required by the CG method to yield an approximation $\mathbf{x}_q^{(n)}$ such that $\sigma_q^{(n)}/\sigma_0^{(n)} < \delta$ is bounded by a number h_δ independent of n ,

$$h_\delta = \left(\ln \frac{\sqrt{M} + 1}{\sqrt{M} - 1} \right)^{-1} \ln \frac{2}{\delta} + 1 \leq \frac{1}{2} \sqrt{M} \ln \frac{2}{\delta} + 1.$$

If (5.1) is the unique information available on the distribution of the eigenvalues of $A^{(n)}$, one cannot obtain an upper bound better than (5.3). Thus, if the constant M —and then h_δ —is large, the coefficient of $\Phi(A^{(n)}\mathbf{f}^{(n)})$ in the operation count may be large. Also, in this case, linear system (5.2) may be ill-conditioned. However, it is well known that a possible clustering property of the eigenvalues of $A^{(n)}$ would tend to increase the rate of convergence of the CG method applied to problem (5.2) [1, pp. 24–28].

A way to gain such clustering property consists in looking for a good preconditioner of the matrix $A^{(n)}$. More precisely, assume that, associated with the given $A^{(n)}$, there exist $n \times n$ matrices S_n , $n = 1, 2, \dots$, having the following properties:

- (i) S_n are positive definite and have uniformly bounded condition numbers. Moreover, no more than $r\Phi(A^{(n)}\mathbf{f}^{(n)})$ arithmetic operations—where r is a suitable constant—are needed to compute S_n and to solve linear systems $S_n\mathbf{z} = \mathbf{f}^{(n)}$.
- (ii) Chosen a matrix E_n such that $S_n = E_n E_n^T$ and denoted by $\tilde{A}^{(n)}$ the positive definite matrix $E_n^{-1} A^{(n)} E_n^{-T}$, the eigenvalues of $\tilde{A}^{(n)}$ (or, equivalently, of $S_n^{-1} A^{(n)}$) are clustered around 1 or, in other terms, 1 is a proper eigenvalue cluster for $\{\tilde{A}^{(n)}\}$ [39], i.e., for any fixed ε ($0 < \varepsilon < 1$) $\exists k_\varepsilon$ and $v_\varepsilon, v_\varepsilon \geq k_\varepsilon$, such that $\forall n > v_\varepsilon$ at least $n - k_\varepsilon$ eigenvalues of $\tilde{A}^{(n)}$ are in the interval $(1 - \varepsilon, 1 + \varepsilon)$. Moreover, we may have $c(\tilde{A}^{(n)}) \leq c(A^{(n)}) \forall n$.

Now consider the following “preconditioned” linear system

$$\tilde{A}^{(n)}\tilde{\mathbf{x}} = (E_n^{-1} A^{(n)} E_n^{-T})(E_n^T \mathbf{x}) = E_n^{-1} \mathbf{b}^{(n)} = \tilde{\mathbf{b}}^{(n)} \quad (5.4)$$

equivalent to (5.2). Notice that the condition number of $\tilde{A}^{(n)}$ is bounded by a constant independent of n . In fact

$$\lambda_1(\tilde{A}^{(n)}) = \min \frac{\mathbf{z}^T \tilde{A}^{(n)} \mathbf{z}}{\mathbf{z}^T \mathbf{z}} \geq \frac{\lambda_1(A^{(n)})}{\lambda_n(S_n)},$$

$$\lambda_n(\tilde{A}^{(n)}) = \max \frac{\mathbf{z}^T \tilde{A}^{(n)} \mathbf{z}}{\mathbf{z}^T \mathbf{z}} \leq \frac{\lambda_n(A^{(n)})}{\lambda_1(S_n)},$$

and therefore, $c(\tilde{A}^{(n)}) \leq c(A^{(n)})c(S_n)$. This remark and the fact that for all $n > v_\varepsilon$ some of the eigenvalues of $\tilde{A}^{(n)}$ must be in $(1 - \varepsilon, 1 + \varepsilon)$, imply in particular that $\inf_n \lambda_1(\tilde{A}^{(n)}) > 0$.

Now let us apply the CG method to the preconditioned system (5.4) (PCG method). Each step of the method can be implemented so that the main operations are a matrix–vector product $A^{(n)}\mathbf{f}^{(n)}$, and a linear system $S_n\mathbf{z} = \mathbf{f}^{(n)}$ solution (“untransformed” version of the PCG method [1]), and thus it can be performed in at most $(r + 1)\Phi(A^{(n)}\mathbf{f}^{(n)})$ arithmetic operations, i.e., with about the same amount of operations required for each step of the CG method applied to (5.2). (Notice that the conditioning of the linear system $S_n\mathbf{z} = \mathbf{f}^{(n)}$ to be solved at each step of the PCG method, is independent of n .) Moreover, if $\mathbf{x}_q^{(n)}$ is the approximation of $\mathbf{x}^{(n)} = A^{(n)^{-1}}\mathbf{b}^{(n)}$ obtained after q steps of the untransformed PCG method, and $\sigma_q^{(n)} = \|\mathbf{x}_q^{(n)} - \mathbf{x}^{(n)}\|_{A^{(n)}}$, then there exists \tilde{u}_q independent of n , such that $\sigma_q^{(n)}/\sigma_0^{(n)} \leq \tilde{u}_q \ll u_q$. More precisely, by applying Theorem 1.11 in [1] for

$$\tilde{P}_q(\lambda) = \prod_{j: \lambda_j^{(n)} \notin [1-\varepsilon, 1+\varepsilon]} \left(1 - \frac{\lambda}{\lambda_j^{(n)}}\right) T_{q-r_\varepsilon^{(n)}}\left(\frac{1-\lambda}{\varepsilon}\right) / T_{q-r_\varepsilon^{(n)}}\left(\frac{1}{\varepsilon}\right),$$

where $\lambda_j^{(n)} = \lambda_j(\tilde{A}^{(n)})$, $r_\varepsilon^{(n)} = \#\{j: \lambda_j^{(n)} \notin [1 - \varepsilon, 1 + \varepsilon]\}$ and $T_m(\lambda)$ is the Chebyshev polynomial of degree m , it can be shown that, $\forall \mathbf{x}_0^{(n)} \in \mathbb{R}^n$,

$$\frac{\sigma_q^{(n)}}{\sigma_0^{(n)}} \leq 2 \prod_{j \in \mathcal{J}_\varepsilon^{(n)}} \left(\frac{1+\varepsilon}{\lambda_j^{(n)}} - 1\right) \left(\frac{\sqrt{M_\varepsilon} - 1}{\sqrt{M_\varepsilon} + 1}\right)^{q-r_\varepsilon^{(n)}} \quad (q \geq r_\varepsilon^{(n)}),$$

where $\mathcal{J}_\varepsilon^{(n)} = \{j: \lambda_j^{(n)} < 1 - \varepsilon \text{ and } \lambda_j^{(n)} < \frac{1}{2}(1 + \varepsilon)\}$ and $M_\varepsilon = (1 + \varepsilon)/(1 - \varepsilon)$. Thus, as a consequence of (i) and (ii), for $A = \inf_n \lambda_1(\tilde{A}^{(n)})$ and

$$\alpha = \begin{cases} \frac{1+\varepsilon}{A} - 1 & \text{if } A < 1 - \varepsilon \text{ and } A < \frac{1}{2}(1 + \varepsilon), \\ 1 & \text{otherwise,} \end{cases}$$

we have, $\forall n > v_\varepsilon$,

$$\frac{\sigma_q^{(n)}}{\sigma_0^{(n)}} \leq \tilde{u}_q = 2\alpha^{k_\varepsilon} \left(\frac{\sqrt{M_\varepsilon} - 1}{\sqrt{M_\varepsilon} + 1}\right)^{q-k_\varepsilon} \cong \left(\frac{\alpha}{\varepsilon}\right)^{k_\varepsilon} \frac{1}{2^{q-k_\varepsilon-1}} \varepsilon^q \quad (5.5)$$

(use the fact that $r_\varepsilon^{(n)} \leq k_\varepsilon \forall n > v_\varepsilon$). In other words, the PCG method converges superlinearly for large n [1,15,17]. As a consequence of (5.5), if ε is chosen small enough and v_ε is enough great with respect to k_ε , then, for any fixed $n > v_\varepsilon$ and $\delta > 0$, the least number q of steps required by the PCG method to yield an approximation $\mathbf{x}_q^{(n)}$ of $\mathbf{x}^{(n)}$ such that $\sigma_q^{(n)}/\sigma_0^{(n)} < \delta$ is bounded by a number \tilde{h}_δ independent of n and such that $\tilde{h}_\delta \ll h_\delta$,

$$\tilde{h}_\delta = \left(\ln \frac{\sqrt{M_\varepsilon} + 1}{\sqrt{M_\varepsilon} - 1} \right)^{-1} \ln \frac{2\alpha^{k_\varepsilon}}{\delta} + k_\varepsilon + 1 \leq \frac{1}{2} \sqrt{M_\varepsilon} \ln \frac{2\alpha^{k_\varepsilon}}{\delta} + k_\varepsilon + 1.$$

From (5.5) it also follows that the rate of convergence of the PCG method depends, in particular, upon the distribution of the smallest eigenvalues of $\tilde{A}^{(n)}$ (see also [1] and the references therein).

Now given a space \mathcal{L} of $n \times n$ matrices, it is natural to check if the best l.s. fits $\mathcal{L}_{A^{(n)}}$ to the $A^{(n)}$ from \mathcal{L} verify properties (i) and (ii), so that the result in (5.5) holds for $S_n = \mathcal{L}_{A^{(n)}}$. Assume that \mathcal{L} is a space of matrices simultaneously diagonalized by a unitary matrix U , so that, by Proposition 2.4,

$$\mathcal{L}_{A^{(n)}} = U d(U^T (\mathcal{L}_{A^{(n)}})^T \mathbf{v}) d(U^T \mathbf{v})^{-1} U^H \quad (5.6)$$

and, by Theorem 2.11(i) (see also [14,28,33] and the references therein), $\mathcal{L}_{A^{(n)}}$ is positive definite and such that

$$\begin{aligned} 0 < a_{\min} &\leq \lambda_1(A^{(n)}) \leq \lambda_1(\mathcal{L}_{A^{(n)}}), \\ \lambda_n(\mathcal{L}_{A^{(n)}}) &\leq \lambda_n(A^{(n)}) \leq a_{\max}, \\ c(\mathcal{L}_{A^{(n)}}) &\leq c(A^{(n)}) \leq M = \frac{a_{\max}}{a_{\min}} \quad \forall n. \end{aligned} \quad (5.7)$$

Moreover, assume that the matrices U and U^T define fast discrete transforms of complexity $O(n \log_2 n)$. For instance \mathcal{L} can be one of the algebras C_β , τ , \mathcal{H} , \mathcal{K} , η , μ , γ of Section 3 or one of the HAs \mathcal{T} associated with the discrete trigonometric transforms classified by Wang in [40] (see [10,31]). Then property (i) is satisfied, for $S_n = \mathcal{L}_{A^{(n)}}$, if the cost of the computation of the \mathbf{v} -row of $\mathcal{L}_{A^{(n)}}$ is such that

$$\Phi(\mathcal{L}_{A^{(n)}}^T \mathbf{v}) \leq r \Phi(A^{(n)} \mathbf{f}^{(n)}) \quad (5.8)$$

for a suitable constant r (we assume $\Phi(A^{(n)} \mathbf{f}^{(n)}) \geq O(n \log_2 n)$). It is known that (5.8), with $\mathbf{v} = \mathbf{e}_1$, is satisfied for $\mathcal{L} = C_\beta, \tau$ both in the generic case ($A^{(n)}$ arbitrary) and in the Toeplitz case, $A^{(n)} = T^{(n)} = (t_{|i-j|})_{i,j=1}^n$, where $\Phi(T^{(n)} \mathbf{f}^{(n)}) = O(n \log_2 n)$ (see Example 3 in Section 2 and [16]). Proposition 4.2 and Theorem 4.3 let us extend this result to the spaces $\mathcal{L} = \eta, \mu$. In the Toeplitz case, (5.8), with $\mathbf{v} = \mathbf{e}_1$, holds also for $\mathcal{L} = \mathcal{H}$ [8], for $\mathcal{L} = \mathcal{T}$ [6,16,31], and now, by Theorem 4.6, for $\mathcal{L} = \mathcal{K}$. If $\mathcal{L} = \gamma$, condition (5.8) has not yet been verified. As γ is a 1-space only for $n \neq 2 + 4r$ one should prove (5.8) for some vector $\mathbf{v} \neq \mathbf{e}_1$ such that $[G^T \mathbf{v}]_j \neq 0 \forall j$ and $\forall n$, for example, for $\mathbf{v} = \mathbf{e}_1 + \mathbf{e}_n$ (see (3.21) in Section 3).

Let us now investigate property (ii) for $S_n = \mathcal{L}_{A^{(n)}}$. If \mathcal{L} and $A^{(n)}$ are generic, as a direct consequence of Theorem 2.11(i), we can say that *the eigenvalues of $\tilde{A}^{(n)} = E_n^{-1}A^{(n)}E_n^{-T}$ ($\mathcal{L}_{A^{(n)}} = E_nE_n^T$) are clustered around 1 if and only if the eigenvalues of $\mathcal{L}_{A^{(n)}} - A^{(n)}$ are clustered around 0*. This fact is a consequence of the result, holding $\forall n$,

$$\begin{aligned} \frac{1}{a_{\max}} |\beta_j^{(n)}| &\leq \frac{1}{\lambda_n(\mathcal{L}_{A^{(n)}})} |\beta_j^{(n)}| \\ &\leq |\alpha_j^{(n)}| \\ &\leq \frac{1}{\lambda_1(\mathcal{L}_{A^{(n)}})} |\beta_j^{(n)}| \\ &\leq \frac{1}{a_{\min}} |\beta_j^{(n)}|, \quad j = 1, \dots, n, \end{aligned} \quad (5.9)$$

where $\alpha_j^{(n)}$ and $\beta_j^{(n)}$ are the eigenvalues, respectively, of $I - E_n^{-1}A^{(n)}E_n^{-T}$ and $\mathcal{L}_{A^{(n)}} - A^{(n)}$ in nondecreasing order. Inequalities (5.9) can be obtained by applying the Courant–Fischer minimax characterization of the eigenvalues of a real symmetric matrix to $I - E_n^{-1}A^{(n)}E_n^{-T}$ and then by using (5.7). Moreover, one may expect that if the $\mathcal{L}_{A^{(n)}}$ do not have the clustering property (ii), then “generally” no other sequence of matrices from \mathcal{L} can have such property, because the $\mathcal{L}_{A^{(n)}}$ better approximate the $A^{(n)}$ from \mathcal{L} . In fact, in case $A^{(n)} = T^{(n)}$ and $\mathcal{L} = C_\beta, \tau, \mathcal{H}, \mathcal{T}$, it is known that, *under suitable hypothesis on $T^{(n)}$* , the $\mathcal{L}_{T^{(n)}}$ satisfy property (ii) (see [15,31] and the references therein). In the following theorem (Theorem 5.1), this result will be extended to the cases $\mathcal{L} = \eta, \mu, \mathcal{K}$. Also notice that in [33] property (ii) for $S_n = \mathcal{L}_{A^{(n)}}$, $\mathcal{L} = \mathcal{T}$, is proved under the same assumption (5.1) in case $A^{(n)} = T_n^T T_n$, where T_n is a generic Toeplitz matrix. In [33], it is also proved that the cost of computation of the eigenvalues of $\mathcal{L}_{A^{(n)}}$ has the same bound of (5.8) for $A^{(n)} = T_n^T T_n$. Thus, (5.5) holds for $S_n = \mathcal{T}_{T_n^T T_n}$.

Remark 5. In principle $\mathcal{L}_{A^{(n)}}$ could be a new possible preconditioner of $A^{(n)}$ even if \mathcal{L} is a noncommutative group matrix algebra $\mathbb{C}[\mathcal{G}]$, or some other space satisfying condition (*) in Section 2, because Theorem 2.11 (i), and therefore (5.7) and (5.9), hold also for such algebras. For instance, if \mathcal{G} is the dihedral group, then the generic element of $\mathbb{C}[\mathcal{G}]$ has the form

$$\begin{pmatrix} X & JY \\ JY & X \end{pmatrix},$$

where X and Y are circulant matrices of order $n/2$ and Theorem 2.11 lets us conclude that $\mathbb{C}[\mathcal{G}]_{A^{(n)}}$ is positive definite. Thus, in order to prove that $\mathcal{L}_{A^{(n)}}$, for some noncommutative $\mathcal{L} = \mathbb{C}[\mathcal{G}]$, satisfies (ii), it would be sufficient to show that the eigenvalues of $\mathcal{L}_{A^{(n)}} - A^{(n)}$ are clustered around 0.

Let us now consider more in detail the case where the $A^{(n)}$ are Toeplitz matrices for which results (5.3) and (5.5) can effectively hold. Let $\{t_r\}_{r=0}^{+\infty}$ be a sequence of real numbers in the Wiener class, i.e.,

$$\sum_{r=0}^{+\infty} |t_r| < +\infty, \quad (5.10)$$

and assume that its generating function is positive

$$t(\vartheta) \equiv \sum_{r=-\infty}^{+\infty} t_{|r|} e^{ir\vartheta} > 0 \quad \forall \vartheta \in [-\pi, \pi]. \quad (5.11)$$

Set $T^{(n)} = (t_{|i-j|})_{i,j=1}^n$, $n = 1, 2, \dots$. Under condition (5.10) the eigenvalues of $T^{(n)}$ are known to be in the interval $[t_{\min}, t_{\max}]$, where $t_{\min} = \min t(\vartheta)$ and $t_{\max} = \max t(\vartheta)$ (see, for example, [13]); thus, by (5.11), they are all positive ($\forall n$). This remark implies that $\{T^{(n)}\}_{n=1}^{+\infty}$ is a sequence of positive definite matrices satisfying (5.1) for $a_{\min} = t_{\min}$ and $a_{\max} = t_{\max}$. Thus, if we consider the linear system

$$T^{(n)} \mathbf{x} = \mathbf{b}^{(n)} \quad (5.12)$$

and apply the CG method to solve it, by (5.3) which then holds for $M = t_{\max}/t_{\min}$, we can have, in principle, an approximation of $\mathbf{x}^{(n)} = T^{(n)-1} \mathbf{b}^{(n)}$ of arbitrary accuracy in only $O(n \log_2 n)$ arithmetic operations. Moreover, in case of a slow convergence of the method (this may happen if the ratio t_{\max}/t_{\min} is large), we can effectively construct, through suitable sequences of preconditioning matrices S_n satisfying (i) and (ii), a preconditioned linear system

$$\tilde{T}^{(n)} \tilde{\mathbf{x}} = (E_n^{-1} T^{(n)} E_n^{-T})(E_n^T \mathbf{x}) = E_n^{-1} \mathbf{b}^{(n)} = \tilde{\mathbf{b}}^{(n)} \quad (5.13)$$

equivalent to (5.12) such that the rate of convergence of the CG method applied to (5.13) verifies (5.5) (see [15,31] and the references therein). As the following theorem (Theorem 5.1) states, three *new* such sequences are $\{\eta_{T^{(n)}}\}$, $\{\mu_{T^{(n)}}\}$ and $\{\mathcal{K}_{T^{(n)}}\}$. In Theorem 5.1, only property (ii) is shown, because we already know that property (i) is verified (see above where property (i) is investigated for *generic* $A^{(n)}$ satisfying (5.1)). In particular, by Theorem 2.11(i), we have, for $\mathcal{L} = \eta, \mu, \mathcal{K}$,

$$\begin{aligned} 0 < t_{\min} &\leq \lambda_1(T^{(n)}) \leq \lambda_1(\mathcal{L}_{T^{(n)}}), \\ \lambda_n(\mathcal{L}_{T^{(n)}}) &\leq \lambda_n(T^{(n)}) \leq t_{\max}, \\ c(\mathcal{L}_{T^{(n)}}) &\leq c(T^{(n)}) \leq t_{\max}/t_{\min} \quad \forall n. \end{aligned} \quad (5.14)$$

Notice that, by Theorem 2.11, (5.14) actually holds for *any* $*$ -space \mathcal{L} , and then, in particular, for $\mathcal{L} =$ commutative algebra of matrices diagonalized by a unitary transform U and for $\mathcal{L} = \mathbb{C}[\mathcal{G}]$, where \mathcal{G} is any (commutative or noncommutative) group.

Theorem 5.1. Let $\{t_r\}_{r=0}^{+\infty}$ be a sequence of real numbers satisfying (5.10) and set $T^{(n)} = (t_{|i-j|})_{i,j=1}^n$. If $\mathcal{L} \in \{\eta, \mu, \mathcal{K}\}$, then the eigenvalues of $\mathcal{L}_T(n) - T^{(n)}$ are clustered around 0. Moreover, if (5.11) is verified, then the same conclusion holds for the matrices $I - \mathcal{L}_{T^{(n)}}^{-1} T^{(n)}$.

Proof. For the sake of simplicity, set $T = T^{(n)}$. Then fix a number $N, n > 2N$. Let $W^{(N)}$ and $E^{(N)}$ denote the $n \times n$ matrices

$$\begin{aligned} [W^{(N)}]_{ij} &= \begin{cases} [(C_{-1})_T - T]_{ij}, & i, j \leq n - N, \\ 0, & \text{otherwise,} \end{cases} \\ [E^{(N)}]_{ij} &= \begin{cases} 0, & i, j \leq n - N, \\ [(C_{-1})_T - T]_{ij}, & \text{otherwise,} \end{cases} \\ i, j &= 1, \dots, n \quad ([(C_{-1})_T - T]_{ij} = -s_{|i-j|}^+ |i - j|/n). \end{aligned}$$

Then

$$\mu_T - T = (C_{-1})_T + JR_{\mu,T} - T = E^{(N)} + (W^{(N)} + JR_{\mu,T}). \quad (5.15)$$

Notice that $E^{(N)}$ has at least $n - 2N$ null eigenvalues ($\text{rank } E^{(N)} \leq 2N$), and that $\mu_T - T$, $E^{(N)}$ and $W^{(N)} + JR_{\mu,T}$ are all real symmetric matrices. Now we prove that, for any fixed $\varepsilon > 0$, there exist N_ε and $v_\varepsilon \geq 2N_\varepsilon$ such that

$$\|W^{(N_\varepsilon)} + JR_{\mu,T}\|_1 < \varepsilon \quad \forall n > v_\varepsilon, \quad (5.16)$$

where $\|\cdot\|_1$ is the matrix 1-norm. As a consequence of this fact and of identity (5.15) for $N = N_\varepsilon$, we shall have that for all $n > v_\varepsilon$ at least $n - 2N_\varepsilon$ eigenvalues of $\mu_T - T$ are in $(-\varepsilon, \varepsilon)$ [41, pp. 101 and 102]. Moreover, if $t_{\min} > 0$, then, by (5.9) with $A^{(n)} = T^{(n)}$, $a_{\min} = t_{\min}$ and $\mathcal{L} = \mu$, we shall also obtain the clustering around 0 of the eigenvalues of $I - \mu_T^{-1} T$. Let us state upper bounds for $\|W^{(N)}\|_1$ and $\|JR_{\mu,T}\|_1$:

$$\|W^{(N)}\|_1 \leq \frac{2}{n} \sum_{j=1}^{n-N-1} j |s_j^+| \leq 2 \sum_{j=N+1}^{n-1} |t_j| + \frac{2}{n} \sum_{j=1}^N j |t_j|. \quad (5.17)$$

Regarding $\|JR_{\mu,T}\|_1$, by Corollary 4.4, for n even we have

$$\begin{aligned} \|JR_{\mu,T}\|_1 &\leq 2 \sum_{k=0}^{\lceil n/4 \rceil - 1} |b_{2k}| + 2 \sum_{k=1}^{\lfloor n/4 \rfloor} |b_{2k-1}| \\ &\leq \frac{4}{n} \left\{ \sum_{k=0}^{\lceil n/4 \rceil - 1} \sum_{j=k+1}^{\lfloor n/4 \rfloor} |s_{2j-1}^+| \right. \\ &\quad \left. + \sum_{k=1}^{\lfloor n/4 \rfloor} \sum_{j=k}^{\lceil n/4 \rceil - 1} |s_{2j}^+| + |t_{n/2}| (\delta_{n/2,0} + \delta_{n/2,e}) \left\lceil \frac{n}{4} \right\rceil \right\} \end{aligned}$$

$$\begin{aligned}
&\leq \frac{4}{n} \left\{ \sum_{k=0}^{\lceil n/4 \rceil - 1} \sum_{j=2k}^{n/2-1} |s_j^+| + |t_{n/2}| \left\lceil \frac{n}{4} \right\rceil \right\} \\
&= \frac{4}{n} \left\{ \sum_{j=0}^{n/2-1} |s_j^+| \left(\left\lfloor \frac{j}{2} \right\rfloor + 1 \right) + |t_{n/2}| \left\lceil \frac{n}{4} \right\rceil \right\} \\
&\leq \frac{4}{n} \left\{ \sum_{j=1}^{n/2-1} j |s_j^+| + \frac{n}{2} |t_{n/2}| \right\} \\
&\leq \frac{4}{n} \sum_{j=1}^{n-1} j |t_j|. \tag{5.18}
\end{aligned}$$

Analogously, for n odd we have

$$\|JR_{\mu,T}\|_1 \leq 2 \sum_{k=0}^{\lfloor (n-1)/4 \rfloor} |b_{2k}| + 2 \sum_{k=1}^{\lceil (n-1)/4 \rceil} |b_{2k-1}| \leq \frac{8}{n} \sum_{j=1}^{n-1} j |t_j|. \tag{5.19}$$

Now let $\varepsilon > 0$ be fixed. Choose N_ε such that $2 \sum_{j=N_\varepsilon+1}^{+\infty} |t_j| < \frac{\varepsilon}{4}$ and set $N = N_\varepsilon$ in (5.17) and in the previous arguments. If $v_\varepsilon, v_\varepsilon \geq 2N_\varepsilon$, is such that, $\forall n > v_\varepsilon$, $\frac{2}{n} \sum_{j=1}^{N_\varepsilon} j |t_j| < \frac{\varepsilon}{4}$ and $\frac{8}{n} \sum_{j=1}^{n-1} j |t_j| < \frac{\varepsilon}{2}$ (the sequence $\frac{1}{n} \sum_{j=1}^{n-1} j |t_j|$ tends to become 0 if (5.10) holds [6]), then, by (5.17) and (5.18) or (5.19), we have thesis (5.16). The proof for $\mathcal{L} = \eta, \mathcal{K}$ is similar. \square

Remark 6. Proceeding as in [30] and using, in particular, the linearity of the operator $A \rightarrow \mathcal{L}_A$, one can extend the result in Theorem 5.1 to sequences $\{t_r\}_{r=0}^{+\infty}$, $t_r = \frac{1}{2\pi} \int_{-\pi}^{\pi} t(\vartheta) e^{-ir\vartheta} d\vartheta$, where $t(\vartheta)$ is any 2π -periodic continuous real-valued even function, positive in $[-\pi, \pi]$.

All previous results together with Theorem 6.1 and some related experimental data listed in Section 6 let us conclude that $\eta_{T(n)}, \mu_{T(n)}$ and $\mathcal{K}_{T(n)}$ are Toeplitz preconditioners competitive with the best-known.

6. Experimental results

Theorem 2.2 lets us calculate the explicit formulas for $\|\mathcal{L}_T - T\|_{\mathbb{F}}^2$, with $\mathcal{L} \in \{\eta, \mathcal{H}, \mathcal{K}, \mu\}$ and $T = (t_{i-j})_{i,j=1}^n$, as functions of $\|C_T - T\|_{\mathbb{F}}^2$ and $\|(C_{-1})_T - T\|_{\mathbb{F}}^2$. So we are able to list all expressions for $\|\mathcal{L}_T - T\|_{\mathbb{F}}^2$ with $\mathcal{L} \in \{\eta, \mathcal{H}, C, \tau, C_{-1}, \mathcal{K}, \mu\}$. The algebra τ is included as the typical algebra associated to real Jacobi trigonometric transforms [31]. Recall [6,16] that τ_T is the matrix of τ whose entries $(1, i)$ are

$$Z^{(n/2)} = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 & \cdot & \cdot \\ 0 & 2 & 0 & 2 & 0 & 2 & \cdot & \cdot \\ 1 & 0 & 3 & 0 & 3 & 0 & \cdot & \cdot \\ 0 & 2 & 0 & 4 & 0 & 4 & \cdot & \cdot \\ 1 & 0 & 3 & 0 & 5 & 0 & \cdot & \cdot \\ 0 & 2 & 0 & 4 & 0 & 6 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

with the last row equal to

$$\begin{bmatrix} 0 & 1 & 0 & 2 & 0 & 3 & \cdots & \frac{n-4}{4} & 0 & \frac{n}{8} \end{bmatrix} \quad \left(\frac{n}{2} \text{ even}\right),$$

$$\begin{bmatrix} \frac{1}{2} & 0 & \frac{3}{2} & 0 & \frac{5}{2} & 0 & \cdots & \frac{n-4}{4} & 0 & \frac{n}{8} \end{bmatrix} \quad \left(\frac{n}{2} \text{ odd}\right).$$

(For the definition of $B_{\mathcal{L}}$ see Theorem 2.2 and the last formula in (2.15) of Proposition 2.9.) In other words the matrices R_{η} , n even and n odd, and R_{μ} , n odd, are the elements of τ , $\tau_{0,-1}$ and $\tau_{0,1}$ whose first rows are

$$\begin{bmatrix} \frac{n}{2} - 1 & 0 & \frac{n}{2} - 3 & 0 & \cdots \end{bmatrix},$$

$$\begin{bmatrix} \frac{n-1}{2} - 1 & \frac{n-3}{2} - 2 & \cdots \end{bmatrix},$$

$$\begin{bmatrix} \frac{n-1}{2} & 1 & \frac{n-3}{2} & 2 & \cdots \end{bmatrix},$$

respectively.

Theorem 6.1. Let $T = (t_{|i-j|})_{i,j=1}^n$, $t_k \in \mathbb{C}$. The following equalities hold:

$$\|\eta_T - T\|_F^2 = \|C_T - T\|_F^2 - \frac{8}{n^2} \mathbf{s}_{\eta}^H R_{\eta} \mathbf{s}_{\eta},$$

$$\|\mathcal{H}_T - T\|_F^2 = \|C_T - T\|_F^2 - \frac{2}{n} \sum_{i=1}^{\lfloor (n-1)/2 \rfloor} |s_i^-|^2,$$

$$\|C_T - T\|_F^2 = \frac{2}{n} \sum_{i=1}^{\lfloor (n-1)/2 \rfloor} i(n-i) |s_i^-|^2,$$

$$\|\tau_T - T\|_F^2 = \frac{2}{n+1} \left[\sum_{i=1}^{\lfloor (n/2)-1 \rfloor} i(n-i-1) (|t_{i+1}|^2 + |t_{n-i}|^2) \right. \\ \left. + \delta_{n,o} \left(\frac{n-1}{2} \right)^2 |t_{(n+1)/2}|^2 \right],$$

$$\begin{aligned}\|(C_{-1})_T - T\|_F^2 &= \frac{2}{n} \left[\sum_{i=1}^{\lfloor (n-1)/2 \rfloor} i(n-i) |s_i^+|^2 + \delta_{n,e} \frac{1}{2} \left(\frac{n}{2} \right)^2 |s_{n/2}^+|^2 \right], \\ \|\mathcal{H}_T - T\|_F^2 &= \|(C_{-1})_T - T\|_F^2 - \frac{2}{n} \left(\sum_{i=1}^{\lfloor (n-1)/2 \rfloor} |s_i^+|^2 + \delta_{n,e} \frac{1}{2} |s_{n/2}^+|^2 \right), \\ \|\mu_T - T\|_F^2 &= \|(C_{-1})_T - T\|_F^2 - \frac{8}{n^2} \mathbf{s}_\mu^H R_\mu \mathbf{s}_\mu,\end{aligned}$$

where $\delta_{n,o}$ ($\delta_{n,e}$) denotes 1 for n odd (even) and 0 for n even (odd).

Proof. Only the first equality is proved here in detail. The proof can be immediately extended to the second, sixth and seventh equality. For the third one see [18]. The proof of the remaining identities is left to the reader. By Corollary 4.5 we can write

$$\begin{aligned}\|\eta_T - T\|_F^2 &= \|C_T - T + JR_{\eta,T}\|_F^2 \\ &= \|C_T - T\|_F^2 + 2 \operatorname{Re}(C_T - T, JR_{\eta,T}) + \|JR_{\eta,T}\|_F^2,\end{aligned}$$

where $JR_{\eta,T}$ is a matrix of η . Notice that $\eta_T - T$ is orthogonal to η (see property (2.4)) and then $0 = (\eta_T - T, JR_{\eta,T}) = (C_T - T, JR_{\eta,T}) + \|JR_{\eta,T}\|_F^2$. Thus,

$$\|\eta_T - T\|_F^2 = \|C_T - T\|_F^2 - \|JR_{\eta,T}\|_F^2.$$

The thesis follows from a direct calculation of $\|JR_{\eta,T}\|_F^2$ using formulas (4.32) and (4.33). \square

The following experimental data agree with the theoretical results proved in Theorems 3.6, 5.1 and 6.1. In Table 1 are displayed the condition numbers of T and of the preconditioned matrices $\tilde{T}_\mathcal{L} = E_\mathcal{L}^{-1} T E_\mathcal{L}^{-T}$, $\mathcal{L}_T = E_\mathcal{L} E_\mathcal{L}^T$, where $\mathcal{L} = \eta, \mathcal{H}, C, \tau, C_{-1}, \mathcal{K}, \mu$. For some of the test matrices T , graphics displaying the eigenvalues of $\tilde{T}_\mathcal{L}$ are also reported. The behavior of the condition numbers is conforming to expectations of the quoted Theorems. In fact the inequalities

$$c(\tilde{T}_\eta) \leq c(\tilde{T}_\mathcal{H}) \leq c(\tilde{T}_C), \quad c(\tilde{T}_\mu) \leq c(\tilde{T}_\mathcal{K}) \leq c(\tilde{T}_{C_{-1}}),$$

which are the analogous, in terms of condition numbers, of the inequalities involving $\|\mathcal{L}_T - T\|_F$ in Theorem 3.6, are almost everywhere verified. From the first examples (the respective values of t_k , $k = 0, \dots, n-1$, are listed here in the following)

$$\begin{aligned}\text{A: } \frac{1}{2^k}, \quad \text{E: } \frac{\cos k}{(k+1)^{0.5}}, \\ \text{B: } \frac{1}{k+1}, \quad \text{F: } \frac{\cos k}{(k+1)^{0.01}}, \\ \text{C: } \frac{1}{(k+1)^{0.5}}, \quad \text{G: } \frac{1}{|\sin k| + 1},\end{aligned}$$

$$D: \frac{1}{(k+1)^{0.01}}, \quad H: \frac{1}{\log_e(k+1)+1},$$

we see that the circulant-type $\eta_T, \mathcal{H}_T, C_T$ or the (-1) -circulant-type $(C_{-1})_T, \mathcal{H}_T, \mu_T$ preconditioners become better—with respect to condition number—than τ_T if $|t_k| \rightarrow 0$ more slowly than $1/k$. Otherwise τ_T is better (see graphics B16, C16 and Table 1). However, examples

$$\begin{aligned} \text{I, IO: } t_k &= \frac{1}{2\pi} \int_{-\pi}^{\pi} t(\vartheta) e^{-ik\vartheta} d\vartheta, \\ t(\vartheta) &= \frac{15}{\pi^4(3-10x+15x^2)} (\vartheta^2 - x\pi^2)^2, \quad x = 0, \quad 1 - \frac{6}{\pi^2} \\ \left(t_0 = 1; \text{ for } k \geq 1 \right. & \quad \text{I: } (-1)^k 20 \left(\frac{1}{(\pi k)^2} - \frac{6}{(\pi k)^4} \right), \\ & \quad \text{IO: } \frac{(-1)^k 90}{2\pi^4 - 30\pi^2 + 135} \left(\frac{1}{k^2} - \frac{1}{k^4} \right) \Big), \end{aligned}$$

where t_k is a function of a parameter x , show that when $t_1 = 0$ ($x = 1 - (6/\pi^2)$), τ_T becomes less efficient with respect to $\{\eta_T, \mathcal{H}_T, C_T\}$ and/or $\{(C_{-1})_T, \mathcal{H}_T, \mu_T\}$, even if $|t_k| \rightarrow 0$ as $1/k^2$. This agrees with the fact that t_1 is absent only in the expression of $\|\tau_T - T\|_F^2$ (Theorem 6.1). Notice also that in any case where the circulant ((-1) -circulant)-type preconditioners are better than τ_T , the same τ_T is better than the (-1) -circulant (circulant)-type preconditioners.

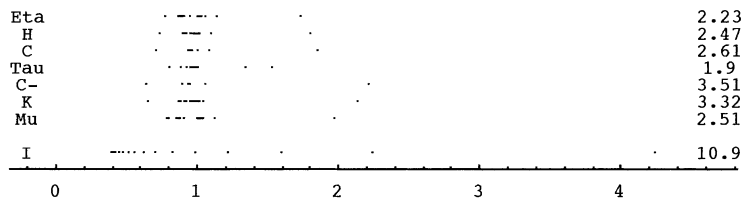
Some suitable preconditioners for ill-conditioned matrices T are analyzed in detail in [13,19,29,34,37]. For such matrices the use of an “improved” optimal preconditioner $\hat{\mathcal{L}}_T$ could be introduced (as in the case $\mathcal{L} = C$ in [37]). Observe that the matrix T in example G is especially ill-conditioned: for instance, if $n = 256$, about $n/2$ of its eigenvalues are less than 0.01.

The fact that $\|\mathcal{L}_T - T\|_F^2$ is a quadratic function of $s_i^- = t_i - t_{n-i}$ ($s_i^+ = t_i + t_{n-i}$) in case $\mathcal{L} \in \{\eta, \mathcal{H}, C\}$ ($\mathcal{L} \in \{C_{-1}, \mathcal{H}, \mu\}$) suggests, in examples E–F, to choose the values $n = 16$ and $n = 19$ in order to show how the dimension n —when the elements t_k change sign—has a significative effect on the performance of the circulant and (-1) -circulant-type preconditioners. In particular, for $n = 16$, t_i and t_{n-i} have opposite sign, and thus $|s_i^+| < |s_i^-|$, for most values of i . This implies that $\|\mathcal{L}_T - T\|_F^2$, for $\mathcal{L} = \mu, \mathcal{H}, C_{-1}$, are dominated by $\|\mathcal{L}_T - T\|_F^2$ with $\mathcal{L} = \eta, \mathcal{H}, C$. The experimental data show an analogous phenomenon in terms of condition numbers: $c(\tilde{T}_{\mathcal{L}})$, with $\mathcal{L} \in \{C_{-1}, \mathcal{H}, \mu\}$ are smaller than $c(\tilde{T}_{\mathcal{L}})$ with $\mathcal{L} \in \{\eta, \mathcal{H}, C\}$.

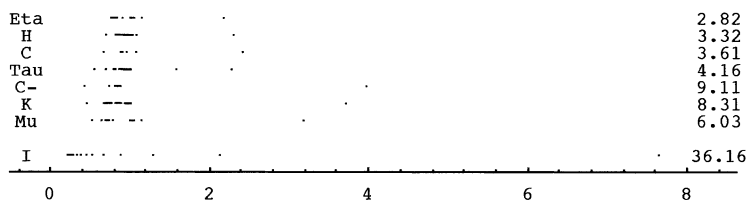
Notice that, if $|s_i^-|$ is small, then T may be viewed as a near circulant matrix, whereas T may be considered like a near (-1) -circulant when $|s_i^+|$ is small.

Graphics : B16, C16, F16, F19

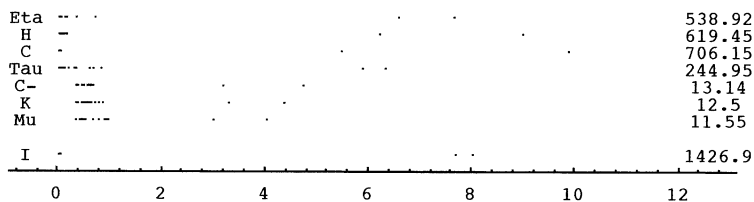
B16: $1/(k+1)$



C16: $1/((k+1)^{0.5})$



F16: $\cos[k]/((k+1)^{0.01})$



F19: $\text{Cos}[k]/((k+1)^{0.01})$

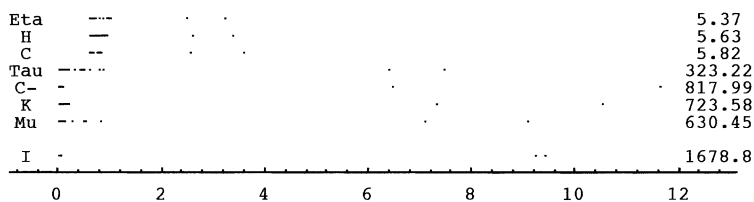


Table 1
Condition numbers of $\tilde{T}_{\mathcal{L}}$ and of T

	A16	B16	C16	D16	E16	E19	F16	F19	G16	G32
η	2.42	2.23	2.82	4.39	5.71	2.52	538.92	5.37	2.98	254.91
\mathcal{H}	2.59	2.47	3.32	4.55	5.75	2.57	619.45	5.63	2.81	251.89
C	2.78	2.61	3.61	5.04	6.26	2.74	706.15	5.82	2.76	255.36
τ	1.35	1.9	4.16	475.99	3.06	3.35	244.95	323.22	35.95	1175.6
C_{-1}	2.78	3.51	9.11	1162.12	2.66	6.44	13.14	817.99	90.59	10141.0
\mathcal{K}	2.59	3.32	8.31	1010.83	2.45	5.99	12.5	723.58	81.57	9248.0
μ	2.36	2.51	6.03	583.41	2.4	5.94	11.55	630.45	44.61	1530.0
I	8.46	10.9	36.16	3464.4	15.76	17.48	1426.9	1678.8	137.73	2452.7

	H16	H32	I16	I016	I32	I032	L16	M16
η	2.05	2.47	759.0	7.8	7896.52	18.6	2.23	37.73
\mathcal{H}	2.3	2.74	819.78	8.11	8703.22	19.1		
C	2.43	2.82	856.99	7.65	9136.55	17.96	2.35	38.64
τ	3.98	5.0	14.02	7.56	33.92	16.93		
C_{-1}	8.18	9.77	868.7	9.95	9172.61	19.69	2.76	39.29
\mathcal{K}	7.65	9.46	769.03	10.22	8549.06	20.6		
μ	5.39	6.52	153.4	9.59	1533.51	19.97	2.39	38.43
I	20.48	33.73	15303.63	58.84	224315.2	235.8	6.28	521.37

The experimental data show that generally the eigenvalues of \tilde{T}_{τ} cluster from the left, while the eigenvalues of \tilde{T}_{η} and \tilde{T}_{μ} cluster from both sides with respect to 1. On the basis of the same data $\tilde{T}_{\mathcal{H}}$, $\tilde{T}_{\mathcal{K}}$ have eigenvalues more regularly spaced than the other preconditioned matrices $\tilde{T}_{\mathcal{L}}$.

Apart from the previous remarks, one must pay attention, however, to the following (experimental) fact: minimizing $\|\mathcal{L}_T - T\|_{\mathbb{F}}^2$ over \mathfrak{H} or \mathfrak{K} (see Theorem 3.6) generally implies minimizing $c(\tilde{T}_{\mathcal{L}})$, but seems also to be a cause of a slower clustering of the eigenvalues of $\tilde{T}_{\mathcal{L}}$ around 1.

In the final examples

$$\text{L: } t_0 = 2, \quad t_k = \frac{1}{(k+1)^{1.1}} - i \frac{1}{(k+1)^{1.1}}, \quad t_{-k} = \bar{t}_k, \quad k \geq 1,$$

$$\text{M: } t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} t(\vartheta) e^{-ik\vartheta} d\vartheta, \quad t(\vartheta) = \frac{12}{7\pi^2} \left(\vartheta - \frac{\pi}{2} \right)^2$$

$$\left(t_0 = 1, \quad t_k = \frac{24(-1)^k}{7(\pi k)^2} - i \frac{12(-1)^k}{7\pi k}, \quad t_{-k} = \bar{t}_k, \quad k \geq 1 \right)$$

we also compare the performance of the two fits to a *Hermitian* Toeplitz matrix $A = (t_{i-j})_{i,j=1}^n$ introduced in Corollary 3.7, $(C + JC)_A$ and $(C_{-1} + JC_{-1})_A$, with

C_A and $(C_{-1})_A$. Obviously, the data in Table 1 are the condition numbers of $\tilde{A}_{\mathcal{L}} = E_{\mathcal{L}}^{-1} A E_{\mathcal{L}}^{-H}$, $E_{\mathcal{L}} E_{\mathcal{L}}^H = \mathcal{L}_A$. Notice that we have no theoretical result on the positive definiteness of $(C + JC)_A$ in case A is positive definite.

For each real test matrix T we have applied the untransformed version of the PCG method (see [1, p. 49]) to solve the systems $T\mathbf{x} = [1 \ 0 \ \cdots \ 0]^T$ (Table 2) and $T\mathbf{x} = [1 \ 1 \ \cdots \ 1]^T$ (Table 3), each one preconditioned by η_T , \mathcal{H}_T , C_T , τ_T , $(C_{-1})_T$, \mathcal{K}_T , μ_T and I , respectively. The solution of the first system defines T^{-1} via Gohberg–Semencul-type formulas (see [23] and the references therein). The second system is often used in the literature to test Toeplitz preconditioners [9,12,13,16]. We report the minimum number k of iterations required to satisfy the condition $\|T\mathbf{x}_k - \mathbf{b}\|_2 / \|\mathbf{b}\|_2 \leq 10^{-7}$, where \mathbf{x}_k is the k th approximation of $T^{-1}\mathbf{b}$ ($\mathbf{x}_0 = \mathbf{0}$). For the τ_T case, when n is a power of 2 greater than 32, the dimension of T is assumed to be $n - 1$ (so that sine transforms can be computed via efficient FFT algorithms). We have also considered the relative errors $\|\mathcal{L}_T - T\|_F / \|T\|_F$, $\mathcal{L} = \eta, \mathcal{H}, C, \tau, C_{-1}, \mathcal{K}, \mu$. These values are calculated by using the formulas of Theorem 6.1. They may be useful, of course, in the effective choice of the best optimal preconditioner and can be computed in at most $O(n \log n)$ steps.

The iterations count in the tables essentially confirms all remarks following from Table 1 and from the graphics. In particular, it is clear that each one of the three sets $\{\tau_T\}$, $\{\eta_T, \mathcal{H}_T, C_T\}$ and $\{(C_{-1})_T, \mathcal{K}_T, \mu_T\}$ can perform better than the other two and that this same set is often recognizable a priori by comparing the \mathcal{L}_T relative errors. Moreover, while Table 2 seems to state that the circulant ((-1)-circulant)-type preconditioned systems converge at the same rate for large n , all examples in Table 3 seem to show that the best optimal preconditioner should be persymmetric (not only symmetric) like T . In fact, in this last table, η_T and μ_T (as C_T and $(C_{-1})_T$) always perform better than \mathcal{H}_T and \mathcal{K}_T , respectively. Notice that in examples I and I0 of Table 3 μ_T performs better (at least for large n), than τ_T even if the τ_T relative error is smaller. We have applied the PCG method also to the system $T\mathbf{x} = [1 \ -1 \ 1 \ -1 \ \cdots]^T$, T as in I, observing a similar conclusion for η_T : for example, if $n = 256$, η_T and τ_T require, respectively, 13 and 20 iterations. One should consider the fact that the efficiency of the preconditioner depends on the form of \mathbf{b} .

Of course from a good preconditioner one also expects that if the condition $\|T\mathbf{x}_k - \mathbf{b}\|_2 / \|\mathbf{b}\|_2 \leq 10^{-7}$ is satisfied, then \mathbf{x}_k is effectively a good approximation of $T^{-1}\mathbf{b}$. From this last point of view a further study of the optimal preconditioners \mathcal{L}_T , $\mathcal{L} \in \{\eta, \mathcal{H}, C, \tau, C_{-1}, \mathcal{K}, \mu\}$, would be advisable.

Table 2

$$T\mathbf{x} = [1 \ 0 \ \dots \ 0]^T$$

		A 128		256	512		B 128		256	512		C 128		256	512
η	.063	6	.0452	5	5	.1	6	.089	7	7	.13	8	.13	8	8
\mathcal{H}	.064	5	.0454	5	5	.116	7	.09445	7	7	.1477	8	.1427	8	8
C	.0642	5	.0455	5	5	.117	7	.09449	7	7	.1478	8	.14272	8	8
τ	.032	4	.022	4	3	.12	7	.1	7	7	.33	9	.31	9	9
C_{-1}	.0642	5	.0455	5	5	.1635	7	.1248	8	8	.4626	8	.43237	9	9
\mathcal{H}	.064	5	.0454	5	5	.1634	7	.1247	7	8	.4625	9	.43234	9	9
μ	.063	6	.0452	5	5	.13	7	.1	7	7	.33	9	.31	9	9
I		24		24	24		25		30	34		35		46	56
		D 128		256	512		E 129		132		F 129		132		
η	.004	8	.0041	9	9	.4464	11	.1426	9	.80721	61	.021996	10		
\mathcal{H}	.00446	8	.0045414	9	9	.4465	11	.14265	9	.80727	49	.021997	10		
C	.00447	9	.0045419	8	9	.4466	11	.1427	9	.8074	39	.022	10		
τ	.56	49	.56	48	49	.32	10	.32	10	.56	46	.56	45		
C_{-1}	.8114	28	.81124	33	38	.1482	10	.4474	11	.07899	12	.8109	39		
\mathcal{H}	.8112	46	.81121	44	44	.14816	10	.4473	11	.07898	13	.8108	49		
μ	.57	35	.57	37	41	.14812	9	.4472	11	.07897	12	.8107	60		
I		53		75	105		31		31		53		51		
		G 256		H 128	512		I 32		128		I0 32		128		256
η	.161961	133	.075	7	7	.15	23	.083	55	.16	15	.09	23	.064	28
\mathcal{H}	.161966	133	.0822	7	8	.163	27	.0844	72	.174	15	.0922	23	.06572	28
C	.16197	133	.08226	7	8	.164	27	.0846	75	.175	14	.0924	22	.06577	28
τ	.57	> 275	.43	9	10	.088	16	.046	27	.13	13	.072	22	.051	27
C_{-1}	.7995	257	.6237	10	11	.168	27	.0847	75	.183	14	.0927	22	.0658	28
\mathcal{H}	.7994	272	.6236	10	11	.166	27	.0845	72	.182	15	.0926	23	.0657	27
μ	.56	245	.44	9	10	.15	23	.082	52	.16	14	.089	23	.064	28
I		143		25	39		57		> 128		34		> 128		> 276

Table 3
 $T\mathbf{x} = [1 \ 1 \ \dots \ 1]^T$

	A 128	256	512	B 128	256	512	C 128	256	512
η	4	4	3	6	6	6	6	6	6
\mathcal{H}	5	5	4	7	7	7	7	7	7
C	4	4	3	5	5	5	5	5	5
τ	4	3	3	6	6	6	7	7	7
C_{-1}	4	4	3	5	5	5	6	6	6
\mathcal{K}	5	5	4	7	7	7	8	8	8
μ	4	4	3	6	6	6	7	7	7
I	20	19	19	18	21	23	22	28	34

	D 128	256	512	E 129	132	F 129	132
η	5	5	5	7	7	45	7
\mathcal{H}	6	6	6	10	9	45	10
C	4	4	5	7	7	27	7
τ	34	35	34	7	8	27	38
C_{-1}	16	18	20	7	8	9	27
\mathcal{K}	34	34	33	9	10	11	46
μ	17	20	24	7	8	9	35
I	22	28	40	23	23	38	38

	G 256	H 128	512	I 32	128	256	I0 32	128	256
η	35	5	6	18	46		10	14	19
\mathcal{H}	45	7	7	27	76		15	22	27
C	36	5	5	16	38	73	10	14	19
τ	176	8	9	12	20	27	9	13	18
C_{-1}	125	7	8	16	38	73	9	13	17
\mathcal{K}	172	9	10	27	76		13	20	25
μ	166	8	9	10	16	20	10	13	16
I	51	16	24	25	> 148		16	77	168

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