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How real is your matrix? ☆

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Dedicated to Roger A. Horn on the occasion of his 65th birthday

Abstract

For scalars there is essentially just one way to define reality, real part and to measure nonreality. In this paper various ways of defining respective concepts for complex-entried matrices are considered. In connection with this, products of circulant and diagonal matrices often appear and algorithms to approximate additively and multiplicatively with them are devised. Multiplicative structures have applications, for instance, in diffractive optics, preconditioning and fast Fourier expansions.

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1. Introduction

In this paper we look, in a systematic manner, at ways to define reality for a matrix $A \in \mathbb{C}^{p\times n}$, respective measures of nonreality, as well as matrix nearness problems related to these considerations. Motivated by applications, we confine to the square matrix case $p = n$. Applications are clearly behind questions like this since otherwise there are hardly any good reasons to pay particular attention to real matrices if the complex field is in use.

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Real matrices (analogously, pure imaginary) in the standard sense enjoy many properties, such as the symmetric location of their spectra with respect to the real axis. In view of the most fundamental operations, matrix–vector products with real matrices cost half of those performed with complex matrices, yielding a good quantitative criterion for the notion of reality more generally. Saving like this are of importance in applying iterative methods. As emphasized in [5, p. 1109], savings in more demanding computations can be even from three to four times more. Our interest in real matrices, and hence also in measuring nonreality, stems from the idea of rewriting real matrix problems in a complex form [14].

While looking at nonreality, we often encounter products of circulant and diagonal matrices, as well as scalings. Such products arise also in modelling diffractive optical instruments; see the framework proposed in [17,21]. Motivated by this, we consider approximating, both additively and multiplicatively, with products of circulant and diagonal matrices. Additive approximation consists of approximating A in the Frobenius norm with sums $\sum_{j=1}^{k} C_j D_j$, where C_j and D_j are circulant and diagonal matrices, for $1 \leqslant j \leqslant k$. This gives rise to new preconditioning opportunities for dense Toeplitz related linear systems. It can also be used in multiplicative approximation, where we restrict to the unitary case and devise an alternating iteration to approximate with DCD-matrices, i.e., with matrices that are products of two diagonal and one circulant matrix.

The paper is organized as follows. In Section 2 several notions of reality for matrices are collected in terms of conjugations and circular conjugations. Some remarks on complex symmetric unitary matrices are made. In Section 3 we look at various ways to quantify nonreality in a more informative manner than through the standard approach. An aim is at application motivated geometric measures of nonreality, yielding information also on functions of A. Section 4 deals with a number of related matrix nearness problems involving diagonal and circulant matrices. DCD-matrices are paid particular attention to.

2. Definitions of reality for matrices

There are several natural, although quite different notions of reality for matrices, depending on the role, i.e., the vector space in which matrices are viewed. First we consider conjugations on $\mathbb{C}^n$ and then conjugations on $\mathbb{C}^{n\times n}$.

2.1. Conjugations on $\mathbb{C}^n$

The following operator theoretic definition of reality appeared already in the second edition of the classic [8, p. 146] of Halmos. We do not know who initiated this notion.

Definition 2.1. A matrix $A \in \mathbb{C}^{n\times n}$, when regarded as a linear operator on $\mathbb{C}^n$, is said to be real with respect to a conjugation J on $\mathbb{C}^n$ if

$$AJ = JA. \tag{2.1}$$

Recall that a conjugation J is an antilinear[1] operator on $\mathbb{C}^n$ satisfying $J^2 = I$ and

$$(Jx, Jy) = (y, x) \quad \text{for all } x, y \in \mathbb{C}^n, \tag{2.2}$$

[1] An antilinear operator J satisfies $J(x + y) = Jx + Jy$ and $J(\alpha x) = \bar{\alpha} Jx$ for any $\alpha \in \mathbb{C}$ and $x, y \in \mathbb{C}^n$.

where $(\cdot, \cdot)$ is the standard complex inner product [8, p. 145]. Hence J preserves the 2-norm. If τ denotes the standard conjugation operator $\tau x = \bar{x}$ for $x \in \mathbb{C}^n$, then J can be represented as $E\tau$ for a complex symmetric unitary matrix $E \in \mathbb{C}^{n\times n}$. Also the converse holds, i.e., $E\tau$ gives rise to a conjugation whenever E is complex symmetric and unitary. Then (2.1) reads

$$AE = E\overline{A}. \tag{2.3}$$

By [13, Lemma 4.6.9], there exists $U \in \mathbb{C}^{n\times n}$ such that $E = U\overline{U}^{-1}$, where U can be chosen to be unitary by invoking the Takagi decomposition [12, Corollary 4.4.4]. Then we say that U generates the respective conjugation $UU^{\mathrm{T}}\tau$. This allows the condition (2.1) to be written alternatively as

$$U^T\overline{A}\,\overline{U} = U^*AU \tag{2.4}$$

implying that A must be unitarily similar to a real-entried matrix to be real in the sense of Definition 2.1. Equivalently, there exists an orthonormal basis in which A has a real-entried matrix representation.

Example 1. Any Hermitian matrix A is real with respect to an appropriate conjugation. One option is to take the generating U to be a unitary matrix diagonalizing A.

Observe that the cost of checking reality is an $\mathrm{O}(n^2)$ computation at most since a matrix vector product with both sides of (2.3) applied to a random vector followed by taking their difference yields the correct answer with probability one.

The map

$$U \mapsto UU^{\mathrm{T}}$$

from the set of unitary matrices to the set of complex symmetric unitary matrices is onto. We have

$$UU^{\mathrm{T}}\tau = WW^{\mathrm{T}}\tau \tag{2.5}$$

for two unitary matrices U and W if and only if $U^{\mathrm{T}}\overline{W} = U^*W$, i.e., if and only if U^*W is real-entried. Hence $W = UR$ for a real-entried unitary matrix R is a necessary and sufficient condition for (2.5) to hold. These simple remarks prove the following theorem.

Theorem 2.2. *Unitary matrices $U, W \in \mathbb{C}^{n\times n}$ generate the same conjugation $E\tau$ if and only if there exists a unitary matrix $R \in \mathbb{R}^{n\times n}$ such that $W = UR$.*

Corollary 2.3. *A conjugation $E\tau$ with $E \in \mathbb{R}^{n\times n}$ and $E \neq I$ is generated only by a complex-entried unitary matrix.*

For the simplest possible way to generate E we have the following corollary (see also [12, Theorem 4.4.7]).

Corollary 2.4. *Let $E \in \mathbb{C}^{n\times n}$ be unitary and complex symmetric. Then $E = RD(RD)^{\mathrm{T}}$ with a unitary diagonal $D \in \mathbb{C}^{n\times n}$ and a unitary $R \in \mathbb{R}^{n\times n}$.*

Proof. If $Ex = \mathrm{e}^{\mathrm{i}\theta}x$ for a nonzero $x \in \mathbb{C}^n$ and $\theta \in \mathbb{R}$, then conjugating this identity gives $\overline{E}\bar{x} = \mathrm{e}^{-\mathrm{i}\theta}\bar{x}$. By the fact that $\overline{E} = E^{-1}$ we obtain $E\bar{x} = \mathrm{e}^{\mathrm{i}\theta}\bar{x}$. Either $\frac{1}{2}(x + \bar{x})$ or $\frac{1}{2i}(x - \bar{x})$ is nonzero and thereby yields a real-entried eigenvector of E associated with the eigenvalue $\mathrm{e}^{\mathrm{i}\theta}$. Orthogonalizing and continuing in this manner, a real-entried unitary matrix R is obtained diagonalizing E as $E = R\Lambda R^*$. Taking the square root of Λ gives D. $\square$

This yields a way to build complex symmetric unitary matrices of Householder type depending on a small number of parameters providing conjugations that are very inexpensive to apply. For this, take a diagonal matrix $\widetilde{\Lambda}$ such that $I - 2\widetilde{\Lambda}$ has its eigenvalues on the unit circle as follows.

Corollary 2.5. *Suppose* $z_j \in \mathbb{C}$, *for* $1 \leqslant j \leqslant k$, *are located on the circle of radius* $1/2$ *centered at* $1/2$. *If* $r_j \in \mathbb{R}^n$ *are orthonormal, then the matrix*

$$I - 2\sum_{j=1}^{k} z_j r_j r_j^*$$

is complex symmetric and unitary.

The set of complex symmetric unitary matrices is not a group. It can be regarded as a stratified manifold.

Corollary 2.6. *The set of complex symmetric unitary matrices in* $\mathbb{C}^{n\times n}$ *is a real a stratified manifold with the stratum of maximal dimension* $(n^2+n)/2$.

Proof. The set of complex symmetric unitary matrices in $\mathbb{C}^{n\times n}$ is a real a stratified manifold since its elements are given by the matrices E whose entries satisfy the polynomial equations $EE^* = I$ and $E = E^{\mathrm{T}}$.

Consider the set of unitary diagonal matrices having the diagonal entries $\mathrm{e}^{\mathrm{i}\theta_j}$ whose exponents satisfy $0 < \theta_1 < \theta_2 < \cdots < \theta_n < 2\pi$. It is a real manifold of dimension n. Clearly, with Λ varying in this set and with $R \in \mathbb{R}^{n\times n}$ varying among unitary matrices yields a dense subset of complex symmetric unitary matrices trough $R\Lambda R^*$. Let Λ and $\widetilde{\Lambda}$ be such diagonal matrices and suppose both $R, \tilde{R} \in \mathbb{R}^{n\times n}$ are unitary. Then $R\Lambda R^* = \tilde{R}\widetilde{\Lambda}\tilde{R}^*$ if and only if $S = \tilde{R}^* R\Lambda = \widetilde{\Lambda}\tilde{R}^* R$. This forces $\tilde{R}^* R$ to be diagonal and, since it is unitary and real-entried, its diagonal entries are ± 1. Hence R can be chosen such that the first non-zero entry in its each column is positive. With this restriction, we have a one-to-one representation of complex symmetric unitary matrices in a neighborhood of S so that since the dimension of the manifold of real unitary matrices in $\mathbb{R}^{n\times n}$ is $(n^2-n)/2$ (see [18, p. 197]), the claim follows. □

In practice it is of interest that an application of a unitary matrix generating a conjugation consumes a small number of floating point operations. In view of this and Corollary 2.3, one of the most interesting conjugation with a real-entried $E \neq I$ is generated as follows.

Example 2. Take $U = F_n \in \mathbb{C}^{n\times n}$, where F_n is the Fourier matrix [4, p. 32]. Then $E = UU^{\mathrm{T}}$ is the permutation matrix having ones at the positions (1,1) and $(n-j+1, j+1)$, for $j = 1, 2, \ldots, n-1$. In case $A = URU^*$ for a real-entried R, matrix–vector products with A cost essentially the same as those performed with real-entried matrices, once the FFT is invoked.

This example can be viewed in a more general framework, where computation of matrix–vector products is economical.

Theorem 2.7. *Let* $A \in \mathbb{C}^{n\times n}$ *satisfy* (2.3) *with a symmetric permutation matrix* E. *Then a matrix–vector product with* A *costs at most one matrix–vector product with a real-entried matrix plus four inner products in* $\mathbb{C}^n$.

Proof. Build a unitary matrix $U \in \mathbb{C}^{n\times n}$ as follows. If the jth diagonal entry of E is one, then set the jth diagonal entry of U also to be one. Suppose the (k, j)-entry and the (j, k)-entry of E, with $j \neq k$, equal one. Then let the (k, k)-entry and the (j, j)-entry of U be $(1 + i)/2$ and the (j, k)-entry and the (k, j)-entry of U be $(1 - i)/2$. By (2.4) this yields $UU^{\mathrm{T}} = E$ such that $A = URU^*$ with $R \in \mathbb{R}^{n\times n}$. Applying either U or U^* to a vector costs no more than two inner products in $\mathbb{C}^n$. □

Observe that in $\mathbb{C}^{n\times n}$ there are $\binom{n}{k}\left(\frac{n-k}{2}!\right)$ such symmetric permutation matrices having exactly k ones on the diagonal. See [5, p. 1108] for a number of interesting applications involving conjugations of this type.

Later on we need a nearest conjugation in the Frobenius norm $\|\cdot\|_F$. By $\|\cdot\|$ we denote the operator norm while using the standard complex Euclidean metric on $\mathbb{C}^n$.

Theorem 2.8. *Let $A = S + T \in \mathbb{C}^{n\times n}$ with S complex symmetric having the Takagi decomposition $S = U\Sigma U^{\mathrm{T}}$ and T skew-symmetric. Then UU^{T} is a nearest complex symmetric unitary matrix to A in the Frobenius norm.*

Proof. Use the standard inner product $(M, N) = \mathrm{tr}(N^*M)$ on $\mathbb{C}^{n\times n}$ with $M, N \in \mathbb{C}^{n\times n}$. Then the set of complex symmetric matrices is orthogonal to the set of skew-symmetric matrices. Hence the problem of approximating A with a complex symmetric unitary matrix is equivalent to approximating S with a complex symmetric unitary matrix. By the fact that the Frobenius norm is unitarily invariant we can consider minimizing $\|\Sigma - U^*E\overline{U}\|_F$ while E, or equivalently, $U^*E\overline{U}$ varies over the complex symmetric unitary matrices. From this the claim follows. □

To have a purely algebraic conjugation operation not related to the complex Euclidean geometry of $\mathbb{C}^n$, the assumptions of Definition 2.1 need to be relaxed. For this we call an antilinear operator J satisfying merely $J^2 = I$ a *circular conjugation*, i.e., (2.2) is not assumed and therefore J cannot be expected to preserve the 2-norm. This terminology is motivated by [13, p. 478] since a circular conjugation can be represented as $E\tau$ with an invertible matrix $E \in \mathbb{C}^{n\times n}$ satisfying

$$E\overline{E} = I. \tag{2.6}$$

For diagonal matrices this condition leads to unitary matrices. The next most interesting class consists of circulant matrices allowing more variety as follows.

Example 3. Suppose $E = F_n^*\Lambda F_n$ is circulant, where $F_n \in \mathbb{C}^{n\times n}$ is the Fourier matrix and $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. For n even from (2.6) we get the conditions $\lambda_{n-j}\overline{\lambda_{j+2}} = 1$ for $j = 0, 1, \ldots, \frac{n}{2} - 1$ and $|\lambda_1| = 1$.

In terms of a circular conjugation, a natural definition of reality is as follows.

Definition 2.9. A matrix $A \in \mathbb{C}^{n\times n}$, when regarded as a linear operator on $\mathbb{C}^n$, is said to be real with respect to a circular conjugation J on $\mathbb{C}^n$ if

$$AJ = JA. \tag{2.7}$$

Consider (2.6). By [12, Lemma 4.6.9], there exists an invertible $S \in \mathbb{C}^{n\times n}$ such that $E = S\overline{S}^{-1}$ leading to the condition (2.3) which can be written as

$$\overline{S}^{-1}\overline{AS} = S^{-1}AS \tag{2.8}$$

corresponding now to (2.4). This implies that A must be similar to a real-entried matrix to be real in the sense of Definition 2.9. Equivalently, there exists a basis in which A has a real-entried matrix representation.

With conjugations and circular conjugations, a matrix viewed as an antilinear operator on $\mathbb{C}^n$ gives rise to equally natural notions of reality. To Definition 2.1 corresponds the following.

Definition 2.10. A matrix $A \in \mathbb{C}^{n\times n}$, when regarded as an antilinear operator on $\mathbb{C}^n$, is said to be real with respect to a conjugation J on $\mathbb{C}^n$ if

$$A\tau J = JA\tau. \tag{2.9}$$

Let J be represented by $E\tau = UU^{\mathrm{T}}\tau$ for a unitary matrix $U \in \mathbb{C}^{n\times n}$. Then this condition reads

$$A\overline{E} = E\overline{A}, \tag{2.10}$$

i.e.,

$$U^{*}A\overline{U} = U^{\mathrm{T}}\overline{A}U \tag{2.11}$$

and hence A must be unitarily consimilar to a real-entried matrix to be real in the sense of Definition 2.10. Equivalently, there exists an orthonormal basis in which the antilinear operator $A\tau$ has the matrix representation $R\tau$ with $R \in \mathbb{R}^{n\times n}$.

Example 4. By the Takagi decomposition, any complex symmetric matrix is real in the sense of Definition 2.10, with an appropriate U.

Similarly, relaxing the conjugation to be merely a circular conjugation yields an analogous notion of reality.

Definition 2.11. A matrix $A \in \mathbb{C}^{n\times n}$, when regarded as an antilinear operator on $\mathbb{C}^n$, is said to be real with respect to a circular conjugation J on $\mathbb{C}^n$ if

$$A\tau J = JA\tau. \tag{2.12}$$

Let $E = S\overline{S}^{-1}\tau$ be the matrix representation of J. Then the condition (2.12) can be written as

$$\overline{S}^{-1}\overline{A}S = S^{-1}A\overline{S}, \tag{2.13}$$

i.e., A is must be consimilar to a real-entried matrix to be real in the sense of Definition (2.11).

To be real in the sense of Definition 2.9, the trace of A must be real (and the existence of a real Jordan canonical form [12, p. 151] tells whether A is real with respect to some circular conjugation). As opposed to this, Definition 2.11 imposes no such restrictions on A. In fact, there always exists a circular conjugation such that A is real in the sense Definition 2.11, i.e., every matrix is consimilar to a real-entried matrix; see [1] and [11]. This interesting fact makes the notion of reality interpreted in terms of antilinear operator very versatile.

Employing different circular conjugations in the domain and range leads to the respective generalization. For instance, Definition 2.1 then reads as follows.

Definition 2.12. A matrix $A \in \mathbb{C}^{n\times n}$, when regarded as a linear operator on $\mathbb{C}^n$, is said to be real with respect to conjugations J_1, J_2 on $\mathbb{C}^n$ if

$$AJ_1 = J_2A. \tag{2.14}$$

In terms of matrix representations $E_1\tau = U_1U_1^{\mathrm{T}}\tau$ and $E_2\tau = U_2U_2^{\mathrm{T}}\tau$ for J_1 and J_2, with unitary matrices $U_1, U_2 \in \mathbb{C}^{n\times n}$, the condition says that $U_2^*AU_1$ should be real-entried. This is possible if we are allowed to choose the unitary conjugations freely (employ, for example, the singular value decomposition of A). The actual interesting problem of practical importance is to consider when to achieve this in an inexpensive way, for instance, with diagonal unitary matrices. This we look at in Section 4.1.

2.2. Conjugations on $\mathbb{C}^{n\times n}$

Regarding square matrices as elements of the complex vector space $\mathbb{C}^{n\times n}$ leads to another notion of reality as follows.

Definition 2.13. A matrix $A \in \mathbb{C}^{n\times n}$ is said to be real with respect to a conjugation J on $\mathbb{C}^{n\times n}$ if

$$JA = A. \tag{2.15}$$

This was the way reality was defined in the first edition [7, p. 108] of Halmos' book in the special case of J being the Hermitian transposition, i.e., A is real if and only if $A^* = A$. (Observe the change between the first and second editions how reality is defined.) Probably because of this, the splitting of a square matrix into to the sum of its Hermitian and skew-Hermitian parts was called the "Cartesian decomposition" of the matrix [7, p. 108]. Although still in use, in hindsight this term is not completely satisfactory since there are many natural ways to define reality and hence the respective real and imaginary parts to have a "Cartesian decomposition".

In a similar vain, relaxing assumptions on conjugation gives the following definition.

Definition 2.14. A matrix $A \in \mathbb{C}^{n\times n}$ is said to be real with respect to a circular conjugation J on $\mathbb{C}^{n\times n}$ if

$$JA = A. \tag{2.16}$$

The real part of A is then defined by

$$\frac{1}{2}(A + JA) \tag{2.17}$$

and the imaginary part is obtained by subtracting this from A.

Consider a circular conjugation J on $\mathbb{C}^n$ represented as $E\tau$ with $E \in \mathbb{C}^{n\times n}$. Then

$$A \mapsto E\overline{A}\,\overline{E}$$

can be regarded as the related circular conjugation operation on $\mathbb{C}^{n\times n}$ resulting from Definition 2.9 while

$$A \mapsto E\overline{A}E$$

is the related circular conjugation operation on $\mathbb{C}^{n\times n}$ resulting from Definition 2.10. Hence reality in the sense of Definition 2.14 is the most general one including Definitions 2.9 and 2.10 just as special cases.

3. Measures of nonreality and respective matrix splittings

Matrix–vector products with real-entried matrices cost half of those performed with complex matrices, yielding a quantitative measure of nonreality more generally. This is a criterion we apply in splitting matrices below.

Before that, let us first consider more standard measures in terms of Definitions 2.1 and 2.10. (The other definitions of the preceeding section give rise to measures analogously.) The real part of A with respect to Definition 2.1 is the matrix

$$\mathrm{Re}(A) = \frac{1}{2}(A + E\overline{A}\,\overline{E}), \tag{3.1}$$

so that the norm of

$$\mathrm{Im}(A) = A - \mathrm{Re}(A) \tag{3.2}$$

gives rise to a readily computable measure of nonreality of A. Since we are concerned with unitarily invariant norms, this equals the norm of the standard imaginary part $\frac{1}{2}(U^*AU - U^{\mathrm{T}}\overline{A}\,\overline{U})$ of the matrix U^*AU, where U generates $E\tau$.

Example 5. In case of the standard conjugation $E = I$, the matrix (3.1) is used when rounding errors in computations yield a complex-entried answer even though the answer should be real, an example described in [10, p. 2].

In the same way, the real part of A with respect to Definition 2.10 takes the form

$$\frac{1}{2}(A + E\overline{A}E) \tag{3.3}$$

yielding similarly a measure of nonreality of A through the computation of the norm of the imaginary part $A - \mathrm{Re}(A)$. These two measures coincide if and only if E is real-entried.

The measure of nonreality resulting from (3.2) is the straightforward matrix version of the imaginary part computed in the scalar case. To contrast its behaviour, consider the inversion. In the scalar case, for any nonzero $z = x + \mathrm{i}y \in \mathbb{C}$, we have $z^{-1} = \overline{z}/|z|^2$, i.e., there is no (relative) difference in the parts of z and its reciprocal. In the matrix case this is not so since the parts can scale very differently without any usual signs reflecting it. In fact, taking $E = I$ and

$$A = \begin{bmatrix} 1 & t \\ 0 & \mathrm{i} \end{bmatrix} \quad \text{with } t \in \mathbb{R}, \text{ so that } A^{-1} = \begin{bmatrix} 1 & \mathrm{i}t \\ 0 & -\mathrm{i} \end{bmatrix} \tag{3.4}$$

illustrate how the respective sizes of the real and imaginary parts can get completely reversed (when t is large) while $\|A\| = \|A^{-1}\|$ as well as $\|A\|_F = \|A^{-1}\|_F$. It is not indicated by the eigenvalues of A either. This appears to be a feature that should be somehow reflected by a measure of nonreality due to the fact that one is seldom interested in the matrix A alone. In practice functions of A, such as its inverse (in the non-singular case) and its exponential, are sought.

For a geometric point of view, consider the case of A being complex on a small dimensional subspace of $\mathbb{C}^n$. This is obviously the case, for instance, when A is real-entried except one column is complex. To deal with this, consider measuring nonreality modulo small rank perturbations. For simplicity, let $E = I$ and look at

$$\min_{\operatorname{rank}(F)\leqslant k} \|\operatorname{Im}(A - F)\| \tag{3.5}$$

for $1 \leqslant k < n$. Of particular interest is to find F of smallest possible rank such that

$$A = R + F, \tag{3.6}$$

where $R \in \mathbb{R}^{n\times n}$. In this splitting R is said to be the respective real part of A. If the rank of F is small, then A should be though of as being complex on a small dimensional subspace of $\mathbb{C}^n$.

Invoking the Sherman–Morrison–Woodbury formula with the splitting (3.6), the rank behaves in the inversion such that the respective reminder F is of the same rank. Furthermore, suppose $\operatorname{rank}(F) \ll n$ and consider computing matrix–vector products with A. An economical way to do this is to compute matrix–vector products with R and F separately and then form the sum of the vectors. In the inversion savings result analogously, once the Sherman–Morrison–Woodbury formula is applied.

Solving (3.5) and (3.6) can be accomplished in terms of the singular value decomposition of $\operatorname{Im}(A)$.

Theorem 3.1. *Let* $A = X + \mathrm{i}Y \in \mathbb{C}^{n\times n}$ *with* $X, Y \in \mathbb{R}^{n\times n}$. *Then* $A = R + F$ *with* $R \in \mathbb{R}^{n\times n}$ *and* $F \in \mathbb{C}^{n\times n}$ *with* $\operatorname{rank}(F) = \lceil \frac{\operatorname{rank}(Y)}{2} \rceil$.

Proof. Consider a real-entried rank-2 matrix M given in terms of its reduced singular value decomposition as $M = \sigma_1 u_1 v_1^* + \sigma_2 u_2 v_2^*$, where the right and left singular vectors are obviously real-entried. Form $w = \frac{1}{2}((v_1 + v_2) + \mathrm{i}(v_1 - v_2))$ which is of unit length and orthogonal to $\overline{w}$. Because of the construction, we have $M = M[w\overline{w}][w\overline{w}]^* = Mww^* + M\overline{w}w^{\mathrm{T}} = tw^* + \overline{tw^*} = 2\operatorname{Re}(tw^*)$ with $t = Mw$.

With this, let $Y = \sum_{j=1}^{\operatorname{rank}(Y)} \sigma_j u_j v_j^*$ be the reduced singular value decomposition of Y. Without loss of generality, we may assume $\operatorname{rank}(Y)$ to be even. Then use the prescribed construction with each rank-2 matrix $\sigma_{2k-1}u_{2k-1}v_{2k-1}^* + \sigma_{2k}u_{2k}v_{2k}^*$ to have $t_k w_k^*$, for $1 \leqslant k \leqslant \operatorname{rank}(Y)/2$. As a result, $-\mathrm{i}A - \sum_{k=1}^{\operatorname{rank}(Y)/2} t_k w_k^*$ is pure imaginary, from which the claim follows. $\square$

Let us produce an analogous splitting to (3.6) in terms of scaled circulant matrices. By now approximating with circulant matrices, proposed in [22], can be regarded as classical in numerical linear algebra. Motivated by this, we derive a generalized approximation scheme aimed at measuring nonreality geometrically, as well as at other task in numerical linear algebra. To this end, let $\theta \in \mathbb{R}$ be fixed and look at matrices of the form CD with $C \in \mathscr{C}_\theta$, the set of $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant matrices, and $D \in \mathscr{D}$, the set of diagonal matrices. Invoking the FFT, matrix–vector products with such matrices cost at most $\mathrm{O}(n \log n)$ floating point operations.

Regard the rows of a rank-1 matrix as consisting of a fixed row vector multiplied by constants. The analogy with a matrix CD becomes clear once its diagonals are viewed as modulo n. (The main diagonal is numbered as the zeroth and the rightmost as the $(n-1)$th.) The matrix D takes the role of the row vector while the multiplying constants are the entries appearing in C. Then solving

$$\min_{C\in\mathscr{C}_\theta, D\in\mathscr{D}} \|A - CD\|_F \tag{3.7}$$

can be accomplished by computing the best rank-1 approximation to the matrix obtained by permuting the entries of A and multiplied by $\mathrm{e}^{-\mathrm{i}\theta}$ as follows. Let P denote the permutation matrix having ones the diagonal joining the left lower corner with the right upper corner. Let L_A be the lower triangular matrix having as its jth row the $(j-n)$th diagonal of A, augmented with zeros at the right end, for $j=1,2,\ldots,n$. Similarly, let U_A be the strictly upper triangular matrix having as its jth row the jth diagonal of A, augmented with zeros at the left end, for $j=1,2,\ldots,n-1$. With these preliminaries, define $\mathbf{P}_\theta$ on $\mathbb{C}^{n\times n}$ as

$$\mathbf{P}_\theta(A) = P(L_A + \mathrm{e}^{-\mathrm{i}\theta} U_A). \tag{3.8}$$

A 3-by-3 example should clarify this operation.

Example 6. $\mathbf{P}_\theta$ acts on $\mathbb{C}^{3\times 3}$ as

$$\mathbf{P}_\theta\left(\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\right) = \begin{bmatrix} a_{11} & a_{22} & a_{33} \\ a_{21} & a_{32} & 0 \\ a_{31} & 0 & 0 \end{bmatrix} + \mathrm{e}^{-\mathrm{i}\theta}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & a_{13} \\ 0 & a_{12} & a_{23} \end{bmatrix},$$

i.e., first the strictly upper triangular part of A is multiplied by $\mathrm{e}^{-\mathrm{i}\theta}$, then the rows of A are rotated 45 degrees and reorganized to have a square matrix.

With the help of the singular value decomposition, solving (3.7) consists of taking the best rank-1 approximation $\sigma_1 u_1 v_1^*$ to $\mathbf{P}_\theta(A)$ and applying $\mathbf{P}_\theta^{-1}$ to it to have

$$CD = C_\theta(\sqrt{\sigma_1}u_1)\mathrm{diag}(\sqrt{\sigma_1}\overline{v_1}),$$

where $C_\theta(\sqrt{\sigma_1}u_1)$ denotes the $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant matrix having $\sqrt{\sigma_1}u_1$ as its first column.

Proposition 3.2. *Let $M \in \mathbb{C}^{n\times n}$. Then $\mathbf{P}_\theta(M)$ is of rank 1 if and only if $M = CD$ with $C \in \mathscr{C}_\theta$ and $D \in \mathscr{D}$.*

Remark. In view of preconditioning for iteratively solving linear systems, this approach is prone to yield better preconditioners than mere circulant preconditioning [3]. The cost of solving (3.7) to have a preconditioner CD consists of finding approximately the best rank-1 approximation to $\mathbf{P}_\theta(A)$. For this there are efficient high quality software such as `Propack` [19].

Since $\mathbf{P}_\theta$ on $\mathbb{C}^{n\times n}$ is linear and preserves the Frobenius norm, we can conclude that with the prescribed approach we can solve

$$\min_{C_j\in\mathscr{C}_\theta, D_j\in\mathscr{D}} \left\| A - \sum_{j=1}^{k} C_j D_j \right\|_F$$

for any $1 \leqslant k \leqslant n$. When zero is attained, we have a representation of A as the sum of products of $\{\mathrm{e}^{\mathrm{i}\theta}\}$-circulant and diagonal matrices.[2] This can be viewed as a tensor-product type of representation of A in a rotated frame. Because of the properties of $\mathbf{P}_\theta$, the set of those matrices that can be represented as the sum of at most k such products is isomorphic to the set of matrices of rank k at most. There are problems with moderate values of k as follows.

Example 7. In an application arising in electrical impedance tomography (see [15] and references therein) there appear large matrices, after discretizations, of the form $\kappa I + CD$ with $\kappa \in \mathbb{C}$, C

[2] Analogous representations are obtained with matrices of the form HD, where H is restricted to be a circulant-Hankel matrix, i.e., a matrix with cyclically appearing anti-diagonals.

circulant and $D \in \mathscr{D}$. Hence, for such matrices $k = 2$ at most. This makes the preconditioning ideas described in the above remark appealing for linear systems involving $\kappa I + CD$.

With θ fixed, analogously to the proof of Theorem 3.1, we can represent A as

$$A = R_1 + \mathrm{e}^{\mathrm{i}\theta} R_2 + \sum_{j=1}^{k} C_j D_j, \tag{3.9}$$

with $R_1 \in \mathbb{R}^{n\times n}$ lower triangular and $R_2 \in \mathbb{R}^{n\times n}$ strictly upper triangular such that k has the smallest possible value. Again, in case $k \ll n$, matrix–vector products with A can be computed economially by performing them separately with the terms, once the FFT is invoked. Then A can be regarded as almost real when interpreted through the complexity of matrix–vector products.

For further geometric ways to quantify the phenomenon described with the matrix and its inverse in (3.4), and more generally with functions of $A \in \mathbb{C}^{n\times n}$, look at the double commutant

$$\mathscr{K}(A; I) = \operatorname{span}\{I, A, A^2, \ldots, A^{n-1}\}$$

of A. For simplicity, consider the standard conjugation $E = I$. Obviously $\mathscr{K}(\overline{A}; I) = \overline{\mathscr{K}(A; I)}$. If we have $\mathscr{K}(\overline{A}; I) = \mathscr{K}(A; I)$, then $A = p(\overline{A})$ for a polynomial p. Then A commutes with $\overline{A}$ and the scalar inversion formula $z^{-1} = \bar{z}/|z|^2$ has a simple analogy as follows, where a real-entried matrix needs to be inverted only once.

Proposition 3.3. *Suppose $A \in \mathbb{C}^{n\times n}$ is invertible and commutes with $\overline{A}$. Then*

$$A^{-1} = \overline{A}(X^2 + Y^2)^{-1},$$

where $X = \frac{1}{2}(A + \overline{A})$ and $Y = \frac{1}{2i}(A - \overline{A})$.

Proof. We have $A\overline{A} = \overline{A}A$ if and only if $XY = YX$. Moreover, $A\overline{A} = X^2 + Y^2$ holds then and therefore $X^2 + Y^2$ is invertible. It then follows that $(X + \mathrm{i}Y)(X - \mathrm{i}Y)(X^2 + Y^2)^{-1} = I$. □

When A commutes with $\overline{A}$, we also obviously have $e^A = e^X \mathrm{e}^{\mathrm{i}Y}$, i.e., most often encountered functions of A can be generated entirely in terms of real-entried matrices. Therefore, when looking at functions of A, the norm of

$$A\overline{A} - \overline{A}A$$

yields an algebraic measure of nonreality of A, while the difference between the subspaces $\mathscr{K}(A; I)$ and $\mathscr{K}(\overline{A}; I)$ can be regarded as measuring the same thing geometrically. Recall that the distance between two subspaces is defined as the norm of $P - Q$, where P and Q are orthogonal projections onto the subspaces [2, p. 202]. On $\mathbb{C}^{n\times n}$ we use the standard inner product $(A, B) = \operatorname{tr}(B^*A)$.

In measuring nonreality of $A \in \mathbb{C}^{n\times n}$, the standard approach is to look at the imaginary part (3.2) with respect to a fixed conjugation, which typically is taken to be $E\tau$ with $E = I$. It is non-standard to allow the conjugation vary, or be even circular. In terms of Definition 2.9 this leads to

$$\inf_{E\overline{E}=I} \|A - E\overline{A}\,\overline{E}\|$$

which appears to be quite an intractable way of measuring nonreality. Consider instead Definition 2.11. As noted in connection with (2.13), we always have

$$\min_{E\overline{E}=I} \|A - E\overline{A}E\| = 0.$$

To solve this, first compute the nullspace of the $\mathbb{C}$-linear operator

$$X \mapsto \overline{A}AX - X\overline{A}A$$

on $\mathbb{C}^{n\times n}$. With its elements X, form $Y = AX + \overline{X}A$ among which find those satisfying $Y\overline{Y} = I$ to have a circular conjugation $Y\tau$ solving the problem.[3]

After these geometric considerations involving conjugations on $\mathbb{C}^n$, let us make some remarks on conjugations on $\mathbb{C}^{n\times n}$. We look at an interesting special case of Definition 2.14 related to the standard Hermitian transposition. For this, let $S \in \mathbb{C}^{n\times n}$ be Hermitian and invertible and define a conjugation on $\mathbb{C}^{n\times n}$ by

$$JA = SA^*S^{-1}. \tag{3.10}$$

This corresponds to using (possibly) an indefinite scalar product in $\mathbb{C}^{n\times n}$; see [6] for its applications. Having $JA = A$ is covered by the following more general result. See also [9].

Theorem 3.4 [20]. *Let $S \in \mathbb{C}^{n\times n}$ be invertible. Then $SA^*S^{-1} = A$ if and only if A is the product of two Hermitian matrices.*

Reality in this sense is thereby seemingly important, for instance, from the point of view of applying iterative methods, provided the factors are know. Respective measures of nonreality can be readily devised.

4. Matrix nearness problems involving circulant and diagonal matrices

Diagonal and circulant matrices appeared regularly in connection with different notions of reality and respective measures of nonreality. In what follows we look at related matrix nearness problems.

4.1. Recovering diagonal scalings of real-entried matrices

A complex multiple of a real-entried matrix

$$\mathrm{e}^{\mathrm{i}\theta}M, \quad \text{with } \theta \in \mathbb{R} \text{ and } M \in \mathbb{R}^{n\times n}, \tag{4.1}$$

is best treated as a pair, i.e., it is beneficial to keep the real matrix separate from the multiplying complex number. All the relevant computations should be performed with M followed then by a multiplication by $\mathrm{e}^{\mathrm{i}\theta}$. In what follows we consider recovering this and more general instances that lead to analogous simplifications.

Proposition 4.1. *Suppose $A = \{r_{jk}\mathrm{e}^{\mathrm{i}\alpha_{jk}}\} \in \mathbb{C}^{n\times n}$. Then the entries of D solving*

$$\max_{D=\mathrm{diag}(\mathrm{e}^{\mathrm{i}\theta_1},\ldots,\mathrm{e}^{\mathrm{i}\theta_n})} \left\| \frac{1}{2}(DA + \overline{D}\,\overline{A}) \right\|_F,$$

satisfy $\tan(2\theta_j) = -\frac{\sum_{k=1}^n r_{jk}^2 \sin(2\alpha_{jk})}{\sum_{k=1}^n r_{jk}^2 \cos(2\alpha_{jk})}$ *for* $1 \leqslant j \leqslant n$.

Proof. Partial differentiate $\|\frac{1}{2}(DA + \overline{D}\,\overline{A})\|_F^2 = \sum_{j=1}^n \sum_{k=1}^n r_{jk}^2 \cos^2(\alpha_{jk} + \theta_j)$ with respect to θ_j and set equal to zero. Use trigonometric formulae to have the claim. □

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[3] Observe that with Theorem 2.8 one can produce a conjugation to approximate a given circular conjugation.

Scaling from the right is solved analogously. Hence with $A \in \mathbb{C}^{n\times n}$ given, look at

$$\max_{D_1,D_2} \left\| \frac{1}{2}(D_1AD_2 + \overline{D}_1\overline{A}\,\overline{D}_2) \right\|_F,$$

where D_1 and D_2 are constrained to be diagonal and unitary. A method to solve this approximately consists of applying Proposition 4.1 consecutively from the left and right. This gives rise to an alternating direction iteration where half of the unknowns are kept fixed while the remaining ones are optimized. Clearly, a single step costs at most $\mathrm{O}(n^2)$ floating point operations, so that an acceptable number of iterations can be preassigned.

4.2. Nearest matrix from $\mathscr{C}\mathscr{D} + \mathscr{F}_k$

Being interested in small rank perturbations of matrices that possess certain desirable properties, we look at matrices of the form $CD + F_k$, where C is circulant, $D \in \mathscr{D}$ and $F_k \in \mathscr{F}_k$, the set of matrices of rank k at most. Since CD is readily invertible, then so is $CD + F_k$, as long as k is small and the Sherman–Morrison–Woodbury formula is invoked. This class includes very familiar matrices.

Example 8. Matrices of the form $\kappa I + F_k$ with $\kappa \in \mathbb{C}$ and $F_k \in \mathscr{F}_k$, such as elementary matrices, are fundamental for matrix computations.

To find a nearest matrix in the Frobenius norm of the form $CD + F_k$ to $A \in \mathbb{C}^{n\times n}$, consider an alternating direction iteration as follows.

Algorithm 1. To approximate $A \in \mathbb{C}^{n\times n}$ with $CD + F_k$:
with an initial guess $F_k^{(0)}$ for F_k and $j = 0$
repeat
  $j = j + 1$
  solve $\min_{C^{(j)}\in\mathscr{C}_0, D^{(j)}\in\mathscr{D}} \|A - F_k^{(j-1)} - C^{(j)}D^{(j)}\|_F$
  solve $\min_{F^{(j)}\in\mathscr{F}_k} \left\|A - C^{(j)}D^{(j)} - F_k^{(j)}\right\|_F$

For this to be of practical interest, a single step should cost at most $O(n^2)$ floating point operations. Therefore, as in solving (3.7), an iterative method to provide approximative small rank approximations must be applied.

4.3. Approximating with the products of circulant and diagonal matrices

The matrix nearness problem (3.7) can be related to the design of diffractive optical systems, where one is interested in factoring matrices as the product of circulant and diagonal matrices [17,21]. Any unitary matrix equals the product of unitary circulant and unitary diagonal matrices [21, Proposition 7]. Hence by invoking the singular value decomposition, any square matrix is the product of circulant and diagonal matrices. Such products with a small number of factors appear frequently in numerical linear algebra, as the following interpretation illustrates.

Example 9. A rank-1 matrix, a basic building block of linear algebra, can readily be given as $D_1\mathbf{1}D_2$, where $\mathbf{1}$ is the circulant matrix having all its entries ones while $D_1, D_2 \in \mathscr{D}$.

Hence it is of interest to set the following definition.

Definition 4.2. $A \in \mathbb{C}^{n\times n}$ is a DCD-matrix if it can be presented as the product of a circulant and two diagonal matrices.

Analogously, CDC-matrices consist of the product of a diagonal and two circulant matrices. If F_n denotes the Fourier matrix and A is a DCD-matrix, then $F_n A F_n^*$ is a CDC-matrix.

Example 10. The so-called CDC-problem consists of finding the factors of a matrix that is known to be a CDC-matrix; see [17, Section 5]. If the DCD-problem is defined analogously, then solving a CDC-problem is equivalent to solving the respective DCD-problem, after performing the similarity transformation with the Fourier matrix.

We view DCD-matrices as potential building blocks for multiplicative approximation, analogously to the way rank-1 matrices are basic building blocks for additive approximation. From the point of view of fast computations and Fourier expansions, attractive orthonormal bases arise in case the number of terms factoring a unitary matrix, possibly approximately, is well below the dimension of the space. Moreover, a unitary matrix factored as the product of circulant and diagonal matrices corresponds to an optical setup absorbing no energy [21, p. 141]. Motivated by these applications, next we consider the fundamental problem of approximating a unitary $U \in \mathbb{C}^{n\times n}$ with such products.

Example 11. Before proceeding, we describe what can go wrong if we merely build on solving $\min_{C\in\mathscr{C},D\in\mathscr{D}} \|U - CD\|_F$. In the 2-by-2 case this gives us for $U = \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix}$ with $\alpha \in \mathbb{R}$ the approximation $C = \operatorname{diag}(\cos\alpha/\sqrt{2}, \cos\alpha/\sqrt{2})$, when $|\cos\alpha| > |\sin\alpha|$, while $D = I$. To approximate U with a unitary matrix, replace C with its nearest circulant unitary by taking $C = I$. But this means that the algorithm is stuck. A reason is that we need complex-entried matrices.

To avoid the stagnation of the preceding example, we force the approximations to move into the complex field by making them accurate for the product of a $\{e^{i\theta}\}$-circulant and a diagonal matrix. To this end, we first solve, with some tolerance, the matrix nearness problem

$$\min_{0\leqslant\theta<2\pi} \min_{C\in\mathscr{C}_\theta, D\in\mathscr{D}} \|U - CD\|_F. \tag{4.2}$$

Observe that for any $\{e^{i\theta}\}$-circulant matrix C we can write $C = \Omega_1^* C_1 \Omega_1$ with a circulant matrix C_1 and

$$\Omega_1 = \operatorname{diag}(1, e^{-i\theta/n}, \ldots, e^{-i\theta(n-1)/n}),$$

so that CD realizing (4.2) is a DCD-matrix. This can be used as an initial guess assuming the factors are unitary, otherwise replace them with their nearest unitaries without changing the structure. The actual iteration then proceeds as follows.

With an initial guess $\widehat{D}_0 C_0 D_0$ to approximate U, solve

$$\min_{C\in\mathscr{C}_0, D\in\mathscr{D}} \|\widehat{D}_0^{-1} U D_0^{-1} C_0^{-1} - DC\|_F \tag{4.3}$$

and put $\widehat{D}_1 C_1 D_1 = \widehat{D}_0 DCC_0 D_0$, after possibly replacing D and C with their nearest unitaries without changing the structure. Then reverse the roles of C and D and solve

$$\min_{C \in \mathscr{C}_0, D \in \mathscr{D}} \|C_1^{-1} \widehat{D}_1^{-1} U D_1^{-1} - CD\|_F \tag{4.4}$$

and put $\widehat{D}_2 C_2 D_2 = \widehat{D}_1 C_1 C D D_1$, after possibly replacing C and D with their nearest unitaries without changing the structure. This DCD-matrix then approximates U.

Observe that the minimization problem (4.3) is solved similarly to the way (4.4) is solved by introducing the linear operator corresponding to (3.8). Hence these steps can then be repeated to have the following alternating direction iteration.

Algorithm 2. To approximate unitary $U \in \mathbb{C}^{n\times n}$ with unitary DCD-matrix:
with an initial guess $\widehat{D}_0 C D_0$ for U
repeat
solve $\min_{C \in \mathscr{C}_0, D \in \mathscr{D}} \|\widehat{D}_0^{-1} U D_0^{-1} C_0^{-1} - DC\|_F$
replace C and D by nearest unitary matrices from $\mathscr{C}_0$ and $\mathscr{D}$
set $\widehat{D}_1 = \widehat{D}_0 D$, $C_1 = CC_0$ and $D_1 = D_0$
solve $\min_{C \in \mathscr{C}_0, D \in \mathscr{D}} \|C_1^{-1} \widehat{D}_1^{-1} U D_1^{-1} - CD\|_F$
replace C and D by nearest unitary matrices from $\mathscr{C}_0$ and $\mathscr{D}$
set $\widehat{D}_0 = \widehat{D}_1$, $C_0 = C_1 C$ and $D_0 = DD_1$

Since this is a fairly nontrivial method, we demonstrate its behaviour with a small dimensional case showing how it recovers unitary DCD-matrices.

Example 12. To illustrate the computations with `Matlab` [16], we took two random unitary diagonal matrices $D_1, D_2 \in \mathbb{C}^{100\times 100}$ and a unitary circulant matrix $C \in \mathbb{C}^{100\times 100}$ and formed $U = D_1 C D_2$. Then we executed Algorithm 2 with the initial guesses $\widehat{D}_0 = C_0 = D_0 = I$, the identity matrix. In Fig. 4.1 we have a convergence plot in the logarithmic scale of the operator

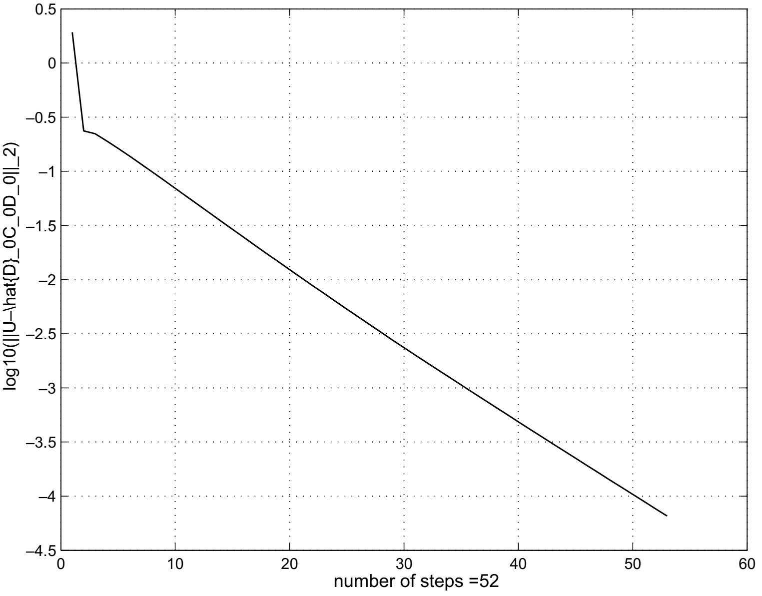

Fig. 4.1. Convergence of Algorithm 2 measured in the $\log_{10}$-scale of $\|U - \widehat{D}_0 C_0 D_0\|_2$ for the problem in Example 12.

norm of $U - \widehat{D}_0 C_0 D_0$. Rounded to four digits, we started with $\|U - I\|_2 = 1.925$ and took 52 repeats. As is to be expected, the convergence is linear.

A crucial step to make Algorithm 2 economical is to have an efficient (iterative) method to produce rank-1 approximations inexpensively in the inner solves. Also FFT should be used in connection with circulant matrices. It remains as an open problem how to extend this method to approximate with several products of DCD-matrices.

5. Conclusions

In this paper we have looked at ways to define reality and real part for matrices, as well as respective measures of nonreality. Geometric aspects were emphasized to have matrix splittings. In connection with this, products of circulant and diagonal matrices often appear and algorithms to approximate additively and multiplicatively with them were devised. Multiplicative structures have applications in diffractive optics, preconditioning and fast Fourier expansions. DCD-matrices were introduced and an alternating direction iteration was devised to approximate unitary matrices with them.

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