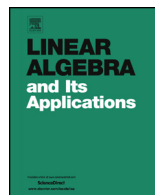




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Symmetry decomposition and matrix multiplication



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ABSTRACT

General matrices can be split uniquely into Frobenius-orthogonal components: a constant row and column sum (type S) part, a vertex cross sum (type V) part and a weight part. We show that for square matrices, the type S part can be expressed as a sum of squares of type V matrices. We investigate the properties of such decomposition under matrix multiplication, in particular how the pseudoinverses of a matrix relate to the pseudoinverses of its component parts. For invertible matrices, this yields an expression for the inverse where only the type S part needs to be (pseudo)inverted; in the example of the Wilson matrix, this component is considerably better conditioned than the whole matrix. We also show a relation between matrix determinants and the weight of their matrix inverses and give a simple proof for Frobenius-optimal approximations with the constant row and column sum and the vertex cross sum properties, respectively, to a given matrix.

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1. Introduction

The interaction between addition and multiplication is one of the basic, but fundamental questions at the root of mathematics, most in evidence in problems of number theory such as the Goldbach conjecture. In matrix algebra, both binary operators are employed in the definition of matrix multiplication. For square matrices M , the determinant is a purely multiplicative proxy, e.g. if $\det M \neq 0$, then there exists a unique inverse matrix M^{-1} with determinant $1/(\det M)$, and the set of all $n \times n$ invertible matrices forms a group under matrix multiplication. However, unlike zero elements in number fields, when $\det M = 0$, there still exists the unique Moore-Penrose inverse M^\dagger of M , with the properties that $M^\dagger M M^\dagger = M^\dagger$, $M M^\dagger M = M$, and both $M M^\dagger$ and $M^\dagger M$ are symmetric. If $\det M \neq 0$ then the pseudoinverse coincides with the inverse.

We can view the determinant as a multiplicative scalar value associated with the square matrix M . As an additive scalar value associated with M , applicable to all $n \times n$ matrices, we consider the average of the entries of M , called the *weight* of the matrix.

Definition 1. Let $M \in \mathbb{C}^{n \times m}$. Then the *weight* of the matrix M is defined by

$$\text{wt } M := \frac{1}{nm} \mathbf{1}_n^T M \mathbf{1}_m.$$

We call M *weightless* if $\text{wt } M = 0$.

Here $\mathbf{1}_n \in \mathbb{C}^n$ is the (column) vector with all entries equal to 1 and $\mathbf{1}_n^T$ denotes the transpose (a row vector). For later use, let $E_{n,m} := \mathbf{1}_n \mathbf{1}_m^T \in \mathbb{C}^{n \times m}$ the matrix with all entries equal to 1, and abbreviate $E_{n,n} := E_n$. The matrix weight is linear, so that for two $n \times m$ matrices M and N and a scalar α , we have that $\text{wt}(\alpha M + N) = \alpha \text{wt } M + \text{wt } N$. Evidently, the weight is not multiplicative, so one can have, e.g., $\text{wt } M \neq 0$ with $\text{wt } M^{-1} = 0$, or $M = N^T N$, with $\text{wt } M \neq (\text{wt } N)^2$. As an example, consider the Wilson matrix [9], denoted by W throughout this paper. This matrix is a mildly ill-conditioned, symmetric positive definite integer matrix, with 2-norm condition number $\kappa_2(W) = \|W\|_2 \|W^{-1}\|_2 \approx 2.98409 \times 10^3$, where $\|A\|_2 = \max_{x \neq 0} \|Ax\|_2 / \|x\|_2$ and $\|x\|_2 = (x^T x)^{1/2}$. It was a favourite of John Todd as a “test matrix” [12–14] and has been used by various authors, for example in [1–4,7]. In [6,8] a quadratic form obstruction was identified to factoring an $n \times n$ symmetric matrix of integers M as $M = Z^T Z$ with Z again an integer matrix. One such factorisation is

$$W = \begin{pmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 3 & 1 & 0 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 & 2 & 2 \\ 1 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 1 & 1 \end{pmatrix} = Z^T Z,$$

where $\det W = 1$, $\text{wt } W = \frac{119}{16} \neq \frac{361}{256} = (\text{wt } Z)^2$. Nevertheless, there are relations between weights and determinants; in Lemma 5 below, we observe that for an invertible $n \times n$ matrix M , the weight of M^{-1} is

$$\text{wt } M^{-1} = \frac{\det(M + E_n) - \det M}{n^2 \det M}.$$

The weight of the inverse matrix can therefore be viewed as the relative change of the determinant of M under perturbation by E_n , averaged over the n^2 matrix entries.

The paper is organised as follows. In Section 2, we introduce the unique Frobenius-orthogonal decomposition of general $n \times m$ matrices into a “type S” part with row sums and column sums equal to 0, a “type V” part with the vertex cross sum property (equivalent, for square matrices, with the co-Latin property), and $E_{n,m}$ multiplied with the weight; see Definition 2 for details regarding these symmetry types. As an application, we identify the weighted type S and the type V matrices closest, in Frobenius norm, to a given matrix (Theorem 4). In Section 3, we observe that square type S matrices can be expressed as sums of squares of type V (co-Latin) matrices and a weight. This representation is not unique, and integer matrices can be expressed in terms of squares of rational matrices with small denominators. We then proceed to consider the pseudoinverses of type V (Section 4) and of type S (Section 5) matrices, showing that these symmetry types are preserved in the process. In Section 6, we investigate how the parts in the decomposition (defined in Section 2) of a matrix and of its pseudoinverse are related. Of course, taking the (pseudo)inverse is not an additive process, so the parts of the pseudoinverse are not simply the pseudoinverses of the parts of the original matrix; nevertheless, we establish some connections. This is particularly successful in the case of an invertible square matrix, where we are able to express the parts of the inverse in terms of the pseudoinverse of the type S part of the matrix, see Theorem 11. In the example of the Wilson matrix, we observe that its type S part is considerably better conditioned than the whole matrix. This suggests a possible application of the present results in numerical linear algebra.

2. $S + V + wE$: a matrix decomposition by symmetry

The square type S matrices with added weight are a subalgebra of the matrix algebra, complemented by the type V matrices to form a superalgebra [10]. The idea of decomposing a real square matrix uniquely over the parts of this superalgebra, revisited in [8], can be extended to rectangular matrices with entries in \mathbb{C} . In the present section we prove the decomposition in generality, emphasising also its orthogonality in the Frobenius inner product, and conclude with an example.

In what follows we use the inner product u^*v for vectors $u, v \in \mathbb{C}^n$, $n \in \mathbb{N}$ throughout; note that, somewhat unusually, this product is linear in the second, conjugate linear in the first factor, but it has the advantage of being conveniently expressed using the matrix

adjoint operation, as we identify \mathbb{C}^n (column vectors) with the matrix space $\mathbb{C}^{n \times 1}$. The orthogonal complements are formed in terms of this inner product.

We also endow the matrix space $\mathbb{C}^{n \times m}$ with the Frobenius inner product $(A, B) := \text{tr } A^*B$ and with the associated norm $\|A\|_F := \sqrt{(A, A)}$ ($A, B \in \mathbb{C}^{n \times m}$). Clearly the above inner product in \mathbb{C}^n coincides with the Frobenius inner product in $\mathbb{C}^{n \times 1}$.

Returning to Definition 1 for the weight of an $n \times m$ matrix $M \in \mathbb{C}^{n \times m}$, the following statements follow by straightforward calculation.

Lemma 1. (a) *The weight $\text{wt} : \mathbb{C}^{n \times m} \rightarrow \mathbb{C}$ is a linear functional generated by the Frobenius inner product with $\frac{1}{nm}E_{n,m}$.*

(b) *The orthogonal projector in $\mathbb{C}^{n \times m}$ onto the subspace spanned by $E_{n,m}$ is*

$$\mathcal{P}_E M = \text{wt } M E_{n,m} \quad (M \in \mathbb{C}^{n \times m}).$$

(c) *The orthogonal projector in $\mathbb{C}^{n \times m}$ onto the subspace of weightless matrices is*

$$\mathcal{P}_0 M = M - \text{wt } M E_{n,m} \quad (M \in \mathbb{C}^{n \times m}).$$

The above considerations give a unique orthogonal decomposition of $n \times m$ matrices into a weightless (i.e. weight 0) part and a multiple of $E_{n,m}$. As an extension of the $S \oplus V$ superalgebra decomposition of square matrices shown in [10] Corollary 2.10, we obtain in the following another orthogonal decomposition of the matrix space, where one of the part contains all matrices with constant row and column sums.

Definition 2. Let $M \in \mathbb{C}^{n \times m}$ and set $w := \text{wt } M$.

(a) *Type S: M has the constant sum property if*

$$M \mathbf{1}_m = m w \mathbf{1}_n, \quad \mathbf{1}_n^T M = n w \mathbf{1}_m^T$$

(i.e. the rows of M sum to $m w$ and the columns of M sum to $n w$); this is equivalent to

$$\mathbf{1}_n^T M u = 0 \quad (u \in \{\mathbf{1}_m\}^\perp), \quad u^T M \mathbf{1}_m = 0 \quad (u \in \{\mathbf{1}_n\}^\perp).$$

(b) *Type V: $M = (M_{i,j})_{i \in \{1, \dots, n\}, j \in \{1, \dots, m\}}$ has the vertex cross sum property if $\text{wt } M = 0$ and*

$$M_{i,j} + M_{k,l} = M_{i,l} + M_{k,j} \quad (i, k \in \{1, \dots, n\}, j, l \in \{1, \dots, m\});$$

the latter condition is equivalent to

$$u^T M v = 0 \quad (u \in \{\mathbf{1}_n\}^\perp, v \in \{\mathbf{1}_m\}^\perp).$$

If $n = m$, then we call matrices with the vertex cross sum property also *co-Latin*.

Remark 1. We collect $n \times m$ matrices with the constant sum property in the vector space $\mathcal{S}_{n,m}$ and matrices with the vertex cross sum property in the vector space $\mathcal{V}_{n,m}$. The equivalence in part (b) follows from the fact that any vector in $\{1_n\}^\perp$ can be written as a linear combination of vectors that have as entries one 1, one -1 and zeros otherwise; indeed, if $u \in \{1_n\}^\perp$, then $u_n = -(u_1 + u_2 + \dots + u_{n-1})$ and

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{n-1} \\ u_n \end{pmatrix} = u_1 \begin{pmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} + (u_1 + u_2) \begin{pmatrix} 0 \\ 1 \\ -1 \\ \vdots \\ 0 \\ 0 \end{pmatrix} + \dots + (u_1 + u_2 + \dots + u_{n-1}) \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ -1 \end{pmatrix}.$$

Square type V matrices are co-Latin in the sense that they have the property that for any $n \times n$ Latin square L , the matrix entries in the positions where L has equal entries sum to the same value; see [8], Theorem 5.1.

Theorem 1. *The matrix $M \in \mathbb{C}^{n \times m}$ has the vertex cross sum property if and only if*

$$M = a1_m^T + 1_nb^*$$

with suitable $a \in \{1_n\}^\perp, b \in \{1_m\}^\perp$.

Proof. Let $M \in \mathcal{V}_{n,m}$. As for any $v \in \{1_m\}^\perp$, we have $Mv \in \{1_n\}^{\perp\perp} = \mathbb{C}1_n$, there is a linear form $f : \{1_m\}^\perp \rightarrow \mathbb{C}$ such that $Mv = 1_nf(v)$. By the Riesz representation theorem in the Hilbert space $\{1_m\}^\perp$, $f(v) = b^*v$ for some representing vector $b \in \{1_m\}^\perp$, so

$$Mv = 1_nb^*v \quad (v \in \{1_m\}^\perp).$$

Now any $x \in \mathbb{C}^m$ is of the form $x = \alpha 1_m + v$ with suitable $\alpha \in \mathbb{C}$ and $v \in \{1_m\}^\perp$, so

$$\begin{aligned} Mx &= \alpha M1_m + 1_nb^*v \\ &= (a1_m^T + 1_nb^*)(\alpha 1_m + v) = (a1_m^T + 1_nb^*)x, \end{aligned}$$

where $a := \frac{1}{m}M1_m$. Note that

$$1_n^T a = \frac{1}{m}1_n^T M1_m = n \text{ wt } M = 0,$$

so $a \in \{1_n\}^\perp$. The converse is evident. \square

As $E_{n,m} \in \mathcal{S}_{n,m}$, Lemma 1 gives a unique orthogonal decomposition of $\mathcal{S}_{n,m}$ into the subspace spanned by $E_{n,m}$ and the space of weightless constant sum matrices $\mathcal{S}_{n,m}^o := \mathcal{P}_0 \mathcal{S}_{n,m}$. Overall we obtain the following decomposition of $n \times m$ matrices.

Theorem 2. *Let $M \in \mathbb{C}^{n \times m}$. Then there are unique $V \in \mathcal{V}_{n,m}$ and $S \in \mathcal{S}_{n,m}^o$ such that $M = V + S + \text{wt } M E_{n,m}$. Specifically,*

$$V = \left(I_n - \frac{1}{n} E_n \right) M \frac{1}{m} E_m + \frac{1}{n} E_n M \left(I_m - \frac{1}{m} E_m \right),$$

$$S = \left(I_n - \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m \right),$$

where I_n, I_m are the $n \times n$ and $m \times m$ unit matrices, respectively.

Proof. Note that $\frac{1}{n} E_n$ is the orthogonal projector onto the subspace spanned by $\mathbf{1}_n \in \mathbb{C}^n$, and consequently $I_n - \frac{1}{n} E_n$ is the orthogonal projector onto the subspace $\{\mathbf{1}_n\}^\perp$. Let

$$a := \frac{1}{m} \left(I_n - \frac{1}{n} E_n \right) M \mathbf{1}_m \quad \text{and} \quad b := \frac{1}{n} \left(I_m - \frac{1}{m} E_m \right) M^* \mathbf{1}_n.$$

Then $a \in \{\mathbf{1}_n\}^\perp$ and $b \in \{\mathbf{1}_m\}^\perp$, so $V := a \mathbf{1}_m^T + \mathbf{1}_n b^* \in \mathcal{V}_{n,m}$ by Theorem 2. Further,

$$\begin{aligned} M - V &= \left(I_n - \frac{1}{n} E_n + \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m + \frac{1}{m} E_m \right) \\ &\quad - \left(I_n - \frac{1}{n} E_n \right) M \frac{1}{m} E_m - \frac{1}{n} E_n M \left(I_m - \frac{1}{m} E_m \right) \\ &= \left(I_n - \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m \right) + \frac{1}{n} E_n M \frac{1}{m} E_m. \end{aligned}$$

The latter term is equal to $\frac{1}{nm} \mathbf{1}_n \mathbf{1}_n^T M \mathbf{1}_m \mathbf{1}_m^T = \text{wt } M E_{n,m} \in \mathcal{S}_{n,m}$; the first term, which we denote by S , is an element of $\mathcal{S}_{n,m}^o$, as

$$\left(I_n - \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m \right) \mathbf{1}_m = 0, \quad \mathbf{1}_n^T \left(I_n - \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m \right) = 0.$$

The uniqueness of the decomposition follows from the fact that $\mathcal{V}_{n,m} \cap \mathcal{S}_{n,m} = \{0\}$. \square

Theorem 3. *The subspaces $\mathcal{V}_{n,m}$ and $\mathcal{S}_{n,m}$ of $\mathbb{C}^{n \times m}$ are orthogonal with respect to the Frobenius inner product $(A, B) := \text{tr } A^* B$.*

Proof. Suppose $S \in \mathcal{S}_{n,m}$ and $V \in \mathcal{V}_{n,m}$. Then $V = a \mathbf{1}_m^T + \mathbf{1}_n b^*$ with suitable $a \in \{\mathbf{1}_n\}^\perp, b \in \{\mathbf{1}_m\}^\perp$ by Theorem 2, so

$$\begin{aligned}
 (S, V) &= \text{tr}(S^* a 1_m^T + S^* 1_n b^*) \\
 &= \text{tr}((S 1_m)^* a + b^* (1_n^T S)^*) \\
 &= \text{tr}(m \overline{\text{wt } S} 1_n^T a + n \overline{\text{wt } S} b^* 1_m) = 0.
 \end{aligned}$$

Further, let $S \in \mathcal{S}_{n,m}$ and $\gamma \in \mathbb{C}$. Then

$$(S, \gamma E_{n,m}) = \gamma \text{tr}(S^* 1_n 1_m^T) = \gamma 1_m^T S^* 1_n = \gamma n m \overline{\text{wt } S} = 0. \quad \square$$

Remark 2. The symmetry types V and S are invariant under taking the adjoint, so that $V \in \mathcal{V}_{n,m} \Rightarrow V^* \in \mathcal{V}_{m,n}$, and $S \in \mathcal{S}_{n,m}^o \Rightarrow S^* \in \mathcal{S}_{m,n}^o$.

Remark 3. The splitting of the matrix space $\mathbb{C}^{n \times m}$ into three mutually Frobenius orthogonal subspaces of Theorem 2 suggests, in the case $n = m$, the attempt to give the subspace of weightless matrices, $\mathcal{P}_0(\mathbb{C}^{n \times n}) = \mathcal{S}_{n,n}^o \oplus \mathcal{V}_{n,n}$, an algebra structure by means of the projected matrix product

$$A \circ B := \mathcal{P}_0(AB) \quad (A, B \in \mathcal{P}_0(\mathbb{C}^{n \times n})).$$

However, it turns out that this product, although bilinear, is not even power associative and hence does not generate a convenient algebra.

Theorems 2 and 3 have the following consequence.

Corollary 1. *The linear mappings $\mathcal{P}_S, \mathcal{P}_V : \mathbb{C}^{n \times m} \rightarrow \mathbb{C}^{n \times m}$ defined as*

$$\begin{aligned}
 \mathcal{P}_S M &:= \left(I_n - \frac{1}{n} E_n \right) M \left(I_m - \frac{1}{m} E_m \right) \\
 \mathcal{P}_V M &:= \left(I_n - \frac{1}{n} E_n \right) M \frac{1}{m} E_m + \frac{1}{n} E_n M \left(I_m - \frac{1}{m} E_m \right) \quad (M \in \mathbb{C}^{n \times m})
 \end{aligned}$$

are the orthogonal projectors onto the subspaces $\mathcal{S}_{n,m}^o$ and $\mathcal{V}_{n,m}$, respectively.

These result lead to the following approximation theorem of general matrices by constant sum matrices of given weight and by matrices with the vertex cross sum property.

Theorem 4. *Let $\theta \in \mathbb{C}$. For $A \in \mathbb{C}^{n,m}$, the matrix*

$$X = \left(I_n - \frac{E_n}{n} \right) A \left(I_m - \frac{E_m}{m} \right) + \theta E_{n,m}$$

is the unique matrix nearest to A in the Frobenius norm with every row sum equal to $m\theta$ and every column sum equal to $n\theta$. Furthermore,

$$Y = A - \left(I_n - \frac{E_n}{n} \right) A \left(I_m - \frac{E_m}{m} \right) - \text{wt } A E_{n,m}$$

is the unique matrix in $\mathcal{V}_{n,m}$ nearest to A in the Frobenius norm.

Proof. For $X \in \mathcal{S}_{n,m}$, we find

$$\begin{aligned} \|X - A\|_F^2 &= \|(\mathcal{P}_S X + \mathcal{P}_V X + \text{wt } X E_{n,m}) - (\mathcal{P}_S A + \mathcal{P}_V A + \text{wt } A E_{n,m})\|_F^2 \\ &= \|\mathcal{P}_S X - \mathcal{P}_S A\|_F^2 + \|\mathcal{P}_V A\|_F^2 + |\text{wt } E - \text{wt } A|^2 \|E_{n,m}\|_F^2. \end{aligned}$$

As we fix the weight $\text{wt } E = \theta$, this expression is clearly uniquely minimised when we take $X = \mathcal{P}_S + \theta E_{n,m}$; the formula in the Theorem follows by Corollary 1.

The matrix Y is evidently the orthogonal projection of A onto $\mathcal{V}_{n,m}$ and hence the nearest matrix to A in that subspace. \square

Example 1. Let $M \in \mathbb{C}^{5 \times 3}$ be the 5×3 matrix given by

$$M = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 1 \\ 4 & 5 & 6 \\ 2 & 1 & 0 \\ 1 & 0 & 3 \end{pmatrix} + \begin{pmatrix} i & 3i & 0 \\ i & i & 0 \\ 2i & i & i \\ 2i & i & 0 \\ i & 0 & i \end{pmatrix}$$

Then M can be decomposed into its type V and type S parts as follows,

$$\begin{aligned} M = V_M + S_M + 2E_{5,3} &= \frac{1}{15} \begin{pmatrix} -6 + 11i & -3 + 8i & 9 - 4i \\ -26 + i & -23 - 2i & -11 - 14i \\ 39 + 11i & 42 + 8i & 54 - 4i \\ -21 + 6i & -18 + 3i & -6 - 9i \\ -16 + i & -13 - 2i & -1 - 14i \end{pmatrix} \\ &+ \frac{1}{15} \begin{pmatrix} -9 - 11i & 3 + 22i & 6 - 11i \\ -4 - i & 8 + 2i & -4 - i \\ -9 + 4i & 3 - 8i & 6 + 4i \\ 21 + 9i & 3 - 3i & -24 - 6i \\ 1 - i & -17 - 13i & 16 + 14i \end{pmatrix} + (2 + i)E_{5,3}. \end{aligned}$$

3. Representations as sums of squares of co-Latin matrices

In this section we focus on square matrices. We abbreviate $\mathcal{S}_n := \mathcal{S}_{n,n}$, $\mathcal{S}_n^o := \mathcal{S}_{n,n}^o$ and $\mathcal{V}_n := \mathcal{V}_{n,n}$.

3.1. From the singular value decomposition

The singular value decomposition of a weightless type S matrix gives rise to the following representation in terms of squares of co-Latin matrices.

Theorem 5. *Let $A \in \mathcal{S}_n^o$. Then there are co-Latin matrices $C_1, \dots, C_r \in \mathcal{V}_n$, with $r \leq n$, such that*

$$A = \sum_{j=1}^r C_j^2 - \frac{\text{tr } A}{n} E_n.$$

Proof. Let $\lambda_1, \dots, \lambda_n \geq 0$ be the eigenvalues of the symmetric matrix A^*A and $u_1, \dots, u_n \in \mathbb{C}^n$ corresponding orthonormal eigenvectors.

Suppose $\lambda_1, \dots, \lambda_r > 0$ and $\lambda_{r+1} = \dots = \lambda_n = 0$. Then v_1, \dots, v_r , defined as

$$v_j = \frac{1}{\sqrt{\lambda_j}} Au_j \quad (j \in \{1, \dots, r\})$$

are orthonormal eigenvectors of AA^* , and the singular value decomposition of A is, considering that the u_j form an orthonormal basis of the orthogonal complement of the null space of A ,

$$A = \sum_{j=1}^r Au_j u_j^* = \sum_{j=1}^r \sqrt{\lambda_j} v_j u_j^*. \tag{3.1}$$

For $j \in \{1, \dots, r\}$, set $a_j := \sqrt{\lambda_j} v_j = Au_j$, $b_j := \frac{1}{n} u_j$ and $C_j := a_j 1_n^* + 1_n b_j^*$. As $A 1_n = 0_n$, which means that 1_n is an eigenvector of A with eigenvalue 0, the orthogonality of the eigenvectors gives $a_j^* 1_n = 0 = b_j^* 1_n$, so the matrix C_j is co-Latin. We then find

$$\begin{aligned} C_j^2 &= a_j 1_n^* a_j 1_n^* + a_j 1_n^* 1_n b_j^* + 1_n b_j^* a_j 1_n^* + 1_n b_j^* a_j b_j^* \\ &= n a_j b_j^* + b_j^* a_j E_n \\ &= Au_j u_j^* + \frac{1}{n} u_j^* Au_j E_n. \end{aligned} \tag{3.2}$$

Therefore

$$A = \sum_{j=1}^r C_j^2 - \frac{1}{n} \sum_{j=1}^r (u_j^* Au_j) E_n.$$

The statement of the theorem now follows upon observing that

$$\sum_{j=1}^r u_j^* Au_j = \sum_{j=1}^r \text{tr}(u_j^* Au_j) = \text{tr } A \sum_{j=1}^r u_j u_j^* = \text{tr } A. \quad \square$$

Remark 4. The matrices C_1, \dots, C_r constructed in the proof of Theorem 5 are not unique; indeed it is apparent that we can, for each $j \in \{1, \dots, r\}$, multiply a_j with a non-zero factor and divide b_j by the same factor without changing the singular value decomposition of A ; this results in different matrices C_j .

Example 2. The part in \mathcal{S}_4^2 of the Wilson matrix W according to the decomposition in Theorem 2 is

$$S_W = \frac{1}{16} \begin{pmatrix} 15 & 11 & -9 & -17 \\ 11 & 23 & -13 & -21 \\ -9 & -13 & 15 & 7 \\ -17 & -21 & 7 & 31 \end{pmatrix}, \tag{3.3}$$

with (to 5 significant figures where relevant) the SVD representation

$$S_W = VDU^* = \begin{pmatrix} -0.41387 & -0.045718 & 0.75936 & \frac{1}{2} \\ -0.55390 & 0.25270 & -0.61590 & \frac{1}{2} \\ 0.32015 & -0.77900 & -0.20164 & \frac{1}{2} \\ 0.64762 & 0.57202 & 0.058178 & \frac{1}{2} \end{pmatrix} \\ \times \begin{pmatrix} 3.9554 & 0 & 0 & 0 \\ 0 & 0.84680 & 0 & 0 \\ 0 & 0 & 0.44784 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ \times \begin{pmatrix} -0.41387 & -0.55390 & 0.32015 & 0.64762 \\ -0.045718 & 0.25270 & -0.77900 & 0.57202 \\ 0.75936 & -0.61590 & -0.20164 & 0.058178 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

Here U is the orthogonal matrix comprised of normalised eigenvectors of S_W , u_1, u_2, u_3, u_4 , $V = U$ and D the diagonal matrix of the singular values of S_W . To construct the vectors a_j and b_j , and so the co-Latin matrices C_j for $1 \leq j \leq 4$ we set

$$a_j := S_W u_j, \quad \text{and} \quad b_j := \frac{1}{4} u_j, \quad \text{with} \quad C_j = a_j 1_4^T + 1_4 b_j^T,$$

so that $C_j^2 = 4u_j u_j^T + \frac{\lambda_j}{4} u_j^T u_j$, yielding $S_W - \frac{21}{16} E_n = C_1^2 + C_2^2 + C_3^2$, where to 5 significant figures

$$C_1 = \begin{pmatrix} -1.7405 & -1.7755 & -1.5570 & -1.4751 \\ -2.2944 & -2.3294 & -2.1109 & -2.0290 \\ 1.1629 & 1.1279 & 1.3464 & 1.4282 \\ 2.4581 & 2.4231 & 2.6416 & 2.7235 \end{pmatrix},$$

$$C_2 = \begin{pmatrix} -0.050144 & 0.024461 & -0.23347 & 0.10429 \\ 0.20256 & 0.27716 & 0.019235 & 0.35699 \\ -0.67109 & -0.59648 & -0.85441 & -0.51665 \\ 0.47296 & 0.54756 & 0.28964 & 0.62739 \end{pmatrix},$$

$$C_3 = \begin{pmatrix} 0.52991 & 0.18610 & 0.28966 & 0.35462 \\ -0.085987 & -0.42980 & -0.32624 & -0.26128 \\ 0.099538 & -0.24428 & -0.14071 & -0.075757 \\ 0.21589 & -0.12792 & -0.024354 & 0.040599 \end{pmatrix}.$$

3.2. From the Smith normal form

Theorem 5 and the approach using the singular value decomposition have the disadvantage that even if the matrix A has integer or rational entries, the co-Latin matrices C_j will in general also have irrational entries. Note that the singular value decomposition shown in equation (3.1) can equivalently be stated in the form

$$A = V \operatorname{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_r}, 0, \dots, 0) U^*,$$

where U and V are the $n \times n$ matrices with columns u_1, \dots, u_n and v_1, \dots, v_n , respectively; here $v_{r+1}, \dots, v_n \in \mathbb{C}^n$ are chosen such as to extend v_1, \dots, v_r to an orthonormal basis of \mathbb{C}^n if $r < n$.

For integer matrices, the singular value decomposition has a natural analogue in the Smith normal form [11]: for any matrix $A \in \mathbb{Z}^{n \times n}$, there are invertible matrices $P, Q \in \mathbb{Z}^{n \times n}$ and positive integers $\alpha_1, \dots, \alpha_r \in \mathbb{N}$ satisfying $\alpha_j | \alpha_{j+1}$ for $j \in \{1, \dots, r-1\}$ (where $r \leq n$) such that

$$A = Q \operatorname{diag}(\alpha_1, \dots, \alpha_r, 0, \dots, 0) P^T. \tag{3.4}$$

Use of this factorisation leads to the following representation in terms of squares of co-Latin matrices with rational entries.

Theorem 6. *Let $A \in \mathbb{Z}^{n \times n} \cap \mathcal{S}_n^o$. Then there are co-Latin matrices*

$$C_1, \dots, C_r \in \frac{1}{n} \mathbb{Z}^{n \times n} \cap \mathcal{V}_n,$$

with $r \leq n$, such that

$$A = \sum_{j=1}^r C_j^2 - \frac{\operatorname{tr} A}{n} E_n.$$

Proof. In the Smith normal form of A given in equation (3.4), let q_1, \dots, q_n be the columns of Q and p_1, \dots, p_n be the columns of P . Then, for any $u \in \mathbb{R}^n$,

$$\begin{aligned}
 Au &= Q \operatorname{diag}(\alpha_1, \dots, \alpha_r, 0, \dots, 0) P^T u \\
 &= (q_1, \dots, q_n) \operatorname{diag}(\alpha_1, \dots, \alpha_r, 0, \dots, 0) \begin{pmatrix} p_1^T u \\ \vdots \\ p_n^T u \end{pmatrix} = \sum_{j=1}^r \alpha_j q_j p_j^T u
 \end{aligned}$$

and therefore $A = \sum_{j=1}^r \alpha_j q_j p_j^T$. Now we observe that $0 = A 1_n = \sum_{j=1}^r \alpha_j q_j p_j^T 1_n$ implies that $p_j^T 1_n = 0$ for all $j \in \{1, \dots, r\}$, since $\alpha_1, \dots, \alpha_r \neq 0$ and q_j, \dots, q_r are linearly independent; similarly,

$$0 = A^T 1_n = \sum_{j=1}^r \alpha_j p_j q_j^T 1_n$$

implies $q_j^T 1_n = 0$ for all $j \in \{1, \dots, r\}$.

Therefore, if we set $a_j := \alpha_j q_j$, $b_j := \frac{1}{n} p_j$ and $C_j := a_j 1_n^T + 1_n b_j^T$, then $C_j \in \frac{1}{n} \mathbb{Z}^{n \times n}$ is co-Latin for all $j \in \{1, \dots, r\}$ and, by equation (3.2)

$$A = \sum_{j=1}^r \alpha_j q_j p_j^T = \sum_{j=1}^r n a_j b_j^T = \sum_{j=1}^r (C_j^2 - b_j^T a_j E_n),$$

giving the representation stated in the theorem since

$$\sum_{j=1}^r b_j^T a_j = \frac{1}{n} \sum_{j=1}^r \alpha_j p_j^T q_j = \frac{1}{n} \sum_{j=1}^r \operatorname{tr}(\alpha_j p_j^T q_j) = \frac{1}{n} \operatorname{tr} \left(\sum_{j=1}^r \alpha_j q_j p_j^T \right) = \frac{\operatorname{tr} A}{n}. \quad \square$$

Example 3. The Smith normal form of the matrix $16S_W$ (see eq. (3.3)) is

$$\begin{aligned}
 16S_W &= Q \operatorname{diag}(\alpha_1, \alpha_2, \alpha_3, 0) P^T \\
 &= \begin{pmatrix} 15 & -28 & 10 & 0 \\ 11 & -20 & 7 & 0 \\ -9 & 17 & -6 & 0 \\ -17 & 31 & -11 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 16 & 0 & 0 \\ 0 & 0 & 96 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 5 & 25 & -31 \\ 0 & -2 & 3 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},
 \end{aligned}$$

where Q and P have determinant 1 and their first three columns are orthogonal to 1_4 . The construction in the proof of Theorem 6 gives the co-Latin matrices

$$C_1 = \frac{1}{4} \begin{pmatrix} 61 & 65 & 85 & 29 \\ 45 & 49 & 69 & 13 \\ -35 & -31 & -11 & -67 \\ -67 & -63 & -43 & -99 \end{pmatrix}, \tag{3.5}$$

$$C_2 = \frac{1}{4} \begin{pmatrix} -1792 & -1794 & -1789 & -1793 \\ -1280 & -1282 & -1277 & -1281 \\ 1088 & 1086 & 1091 & 1087 \\ 1984 & 1982 & 1987 & 1983 \end{pmatrix},$$

$$C_3 = \frac{1}{4} \begin{pmatrix} 3840 & 3839 & 3841 & 3840 \\ 2688 & 2687 & 2689 & 2688 \\ -2304 & -2305 & -2303 & -2304 \\ -4224 & -4225 & -4223 & -4224 \end{pmatrix}$$

satisfying $16S_W = C_1^2 + C_2^2 + C_3^2 - 21 E_4$.

4. Products and pseudoinverses of Type V matrices

In this section we consider products of type V matrices in greater generality. It is known that \mathcal{V}_n forms the odd complement of \mathcal{S}_n in a matrix superalgebra, see [10] Theorem 2.5 (a), so a product of co-Latin matrices is either co-Latin or a constant sum matrix depending on whether the number of factors is odd or even. Here we give an explicit formula for the matrix resulting from a product of several type V matrices. Moreover, as matrices of low rank, type V matrices do not have inverses but we show that their Moore-Penrose pseudoinverses preserve the type V structure.

Lemma 2. *Let $V_j = a_j 1_{n_{j+1}}^T + 1_{n_j} b_j^* \in \mathcal{V}_{n_j, n_{j+1}}$, where $a_j \in \{1_{n_j}\}^\perp \in \mathbb{C}^{n_j}$, $b_j \in \{1_{n_{j+1}}\}^\perp \in \mathbb{C}^{n_{j+1}}$ for $j \in \{1, \dots, N\}$, with $n_1, \dots, n_{N+1} \in \mathbb{N}$. Then*

$$V_1 V_2 \cdots V_{2k+1} = \left(\prod_{j=1}^k n_{2j} b_{2j}^* a_{2j+1} \right) a_1 1_{n_{2k+2}}^T + \left(\prod_{j=1}^k n_{2j+1} b_{2j-1}^* a_{2j} \right) 1_{n_1} b_{2k+1}^* \quad (4.1)$$

if $N = 2k + 1$ is odd, $k \in \mathbb{N}_0$; and

$$V_1 V_2 \cdots V_{2k+2} = \left(\prod_{j=1}^k n_{2j} b_{2j}^* a_{2j+1} \right) n_{2k+2} a_1 b_{2k+2}^* + \left(\prod_{j=1}^k n_{2j+1} b_{2j-1}^* a_{2j} \right) b_{2k+1}^* a_{2k+2} E_{n_1, n_{2k+3}} \quad (4.2)$$

if $N = 2k + 2$ is even, $k \in \mathbb{N}_0$.

Proof. We first observe that the product of two type V matrices takes the form

$$V_1 V_2 = (a_1 1_{n_2}^T + 1_{n_1} b_1^*) (a_2 1_{n_3}^T + 1_{n_2} b_2^*) = n_2 a_1 b_2^* + (b_1^* a_2) E_{n_1, n_3},$$

using the identities $1_{n_2}^T 1_{n_2} = n_2$ and $1_{n_1} 1_{n_3}^T = E_{n_1, n_3}$.

Now we prove identity (4.1) by induction on k . The case $k = 0$ is trivial. Suppose $k \in \mathbb{N}_0$ is such that the claimed identity holds. Then

$$\begin{aligned} V_1 V_2 \cdots V_{2k+3} &= (V_1 V_2 \cdots V_{2k+1})(V_{2k+2} V_{2k+3}) \\ &= \left(\prod_{j=1}^k n_{2j} b_{2j}^* a_{2j+1} \right) (n_{2k+2} b_{2k+2}^* a_{2k+3}) a_1 1_{2k+4}^T \\ &\quad + \left(\prod_{j=1}^k n_{2j+1} b_{2j-1}^* a_{2j} \right) (n_{2k+3} b_{2k+1}^* a_{2k+2}) 1_{n_1} b_{2k+3}^* \\ &= \left(\prod_{j=1}^{k+1} n_{2j} b_{2j}^* a_{2j+1} \right) a_1 1_{n_{2(k+1)+2}}^T + \left(\prod_{j=1}^{k+1} n_{2j+1} b_{2j-1}^* a_{2j} \right) 1_{n_1} b_{2(k+1)+1}^*, \end{aligned}$$

using the identity $1_{n_{2k+2}}^T E_{n_{2k+2}, n_{2k+4}} = n_{2k+2} 1_{2k+4}^T$ for the first term. This completes the proof by induction.

Identity (4.2) then follows by multiplying (4.1) by $V_{2k+2} = a_{2k+2} 1_{n_{2k+3}} + 1_{n_{2k+2}} b_{2k+2}^*$ on the right hand side. \square

By taking all matrices in the product to be the same (square) matrix, we obtain the following formulae for matrix powers of co-Latin matrices.

Corollary 2. *Let $C \in \mathcal{V}_n$ be a co-Latin matrix and $a, b \in \{1_n\}^\perp$ its generating vectors, so $C = a 1_n^T + 1_n b^*$. Then for any non-negative integer $k \in \mathbb{N}_0$, the matrix powers of C satisfy*

$$\begin{aligned} C^{2k+2} &= n^{k+1} (b^* a)^k a b^* + n^k (b^* a)^{k+1} E_n, \\ C^{2k+1} &= n^k (b^* a)^k (a 1_n^T + 1_n b^*). \end{aligned}$$

As a consequence of Theorem 4, we can find the closest constant sum approximant with given weight to the square of a co-Latin matrix as follows.

Corollary 3. *Let C be a co-Latin matrix constructed from vectors a and b , so $C = a 1_n^* + 1_n b^*$ with $a, b \in \{1_n\}^\perp$, and let $\theta \in \mathbb{C}$. Then the unique matrix with every row and column sum equal to θ that is nearest to C^2 in the Frobenius norm is given by*

$$X = n a b^* + \theta E_n,$$

and the Frobenius norm of the difference satisfies

$$\|C^2 - X\| = n |b^* a - \theta|;$$

in particular, the norm of the difference vanishes if and only if $\theta = b^* a$.

Proof. By Theorem 4, the unique constant sum matrix X with weight θ nearest to A is given by

$$X = \left(I_n - \frac{E_n}{n} \right) A \left(I_n - \frac{E_n}{n} \right) + \theta E_n.$$

We know from Corollary 2 that

$$C^2 = n ab^* + (b^* a) E_n,$$

so its weightless constant sum part is given by

$$\mathcal{P}_S C^2 = \left(I_n - \frac{E_n}{n} \right) C^2 \left(I_n - \frac{E_n}{n} \right) = n ab^*$$

(see Corollary 1) and the result follows.

Since $C^2 - X = (b^T a - \theta) E_n$, we find

$$\|C^2 - X\|_F = |b^T a - \theta| \|E_n\|_F = n |b^T a - \theta|. \quad \square$$

For any type V matrix $V \in \mathcal{V}_n$, we now construct the Moore-Penrose pseudoinverse, i.e. the unique matrix V^\dagger such that $V^\dagger V V^\dagger = V^\dagger$, $V V^\dagger V = V$ and both $V V^\dagger$ and $V^\dagger V$ are symmetric. Note that the first two of these equations imply that V^\dagger and V have the same rank.

Theorem 7. Let $V \in \mathcal{V}_{n,m}$ be a type V matrix and $a \in \{1_n\}^\perp$, $b \in \{1_m\}^\perp$ its generating vectors, so $V = a 1_m^T + 1_n b^*$. Set

$$a^\dagger = \frac{b}{n b^* b} \quad \text{and} \quad b^\dagger = \frac{a}{m a^* a};$$

then the matrix $V^\dagger = a^\dagger 1_n^T + 1_m (b^\dagger)^* \in \mathcal{V}_{m,n}$ is the Moore-Penrose pseudoinverse of V .

Proof. By construction, it is evident that $a^\dagger \in \{1_m\}^\perp$, $b^\dagger \in \{1_n\}^\perp$, so V^\dagger is of type V. Using equation (4.1) of Lemma 2 with $k = 1$, we find

$$\begin{aligned} V V^\dagger V &= m (b^\dagger{}^* a) a 1_m^T + n (b^* a^\dagger) 1_n b^* \\ &= m \frac{a^* a}{m a^* a} a 1_m^T + n \frac{b^* b}{n b^* b} 1_n b^T = a 1_m^T + 1_n b^* = V \end{aligned}$$

and

$$\begin{aligned} V^\dagger V V^\dagger &= n (b^* a^\dagger) a^\dagger 1_n^T + m (b^\dagger{}^* a) 1_m b^\dagger{}^* \\ &= n \frac{b^* b}{n b^* b} a^\dagger 1_n^T + m \frac{a^* a}{m a^* a} 1_m b^\dagger{}^* = a^\dagger 1_n^T + 1_m b^\dagger{}^* = V^\dagger. \end{aligned}$$

Further, we note that

$$ab^{\dot{\div}^*} - b^{\dot{\div}}a^* = a \frac{a^*}{ma^*a} - \frac{a}{ma^*a} a^* = 0$$

and

$$a^{\dot{\div}}b^* - ba^{\dot{\div}^*} = \frac{b}{nb^*b} b^* - b \frac{b^*}{nb^*b} = 0;$$

using equation (4.2) of Lemma 2 with $k = 0$, we find that

$$VV^{\dot{\div}} = mab^{\dot{\div}^*} + (b^*a^{\dot{\div}})E_n = mb^{\dot{\div}}a^* + (b^*a^{\dot{\div}})E_n = (VV^{\dot{\div}})^*$$

and

$$V^{\dot{\div}}V = na^{\dot{\div}}b^* + (b^{\dot{\div}^*}a)E_m = nba^{\dot{\div}^*} + (b^{\dot{\div}^*}a)E_m = (V^{\dot{\div}}V)^*. \quad \square$$

Example 4. We consider C_1 from Example 3 (see eq. (3.5)), in the quadratic co-Latin rational expansion for the constant sum equals zero part of the Wilson matrix. Here we have the vector representation $C_1 = a1_n^T + 1_nb^T$, with

$$a = (15, 11, -9, -17)^T, \quad \text{and} \quad b = \left(\frac{1}{4}, \frac{5}{4}, \frac{25}{4}, -\frac{31}{4}\right)^T.$$

Applying Theorem 7 we find that

$$a^{\dot{\div}} = \left(\frac{1}{1612}, \frac{5}{1612}, \frac{25}{1612}, -\frac{1}{52}\right)^T \quad \text{and} \quad b^{\dot{\div}} = \left(\frac{15}{2864}, \frac{11}{2864}, -\frac{9}{2864}, -\frac{17}{2864}\right)^T,$$

whence

$$C_1^{\dot{\div}} = \frac{1}{1154192} \begin{pmatrix} 6761 & 5149 & -2911 & -6135 \\ 9625 & 8013 & -47 & -3271 \\ 23945 & 22333 & 14273 & 11049 \\ -16151 & -17763 & -25823 & -29047 \end{pmatrix}.$$

5. The pseudoinverses of Type S matrices

In addition to giving an explicit formula for the Moore-Penrose pseudoinverse of a type V matrix, Theorem 7 shows that this pseudoinverse is again a type V matrix. In the following we show that the pseudoinverses of (weightless) type S matrices are also of (weightless) type S.

Theorem 8. *Let $S \in \mathcal{S}_{n,m}^o$. Then $S^{\dot{\div}} \in \mathcal{S}_{m,n}^o$.*

Proof. We find

$$S^\dagger 1_n = S^\dagger S S^\dagger 1_n = S^\dagger (S S^\dagger)^* 1_n = S^\dagger S^{\dagger*} S^* 1_n = S^\dagger S^{\dagger*} 0 = 0$$

and similarly

$$\begin{aligned} S^{\dagger*} 1_m &= (S^\dagger S S^\dagger)^* 1_m = S^{\dagger*} S^* S^\dagger 1_m = S^{\dagger*} (S^\dagger S)^* 1_m \\ &= S^{\dagger*} S^\dagger S 1_m = S^{\dagger*} S^\dagger 0 = 0. \quad \square \end{aligned}$$

Theorem 9. *Let $A \in \mathcal{S}_{n,m}$ and $S = \mathcal{P}_S A \in \mathcal{S}_{n,m}^o$, so $A = S + \text{wt } A E_{n,m}$. Then*

$$A^\dagger = \begin{cases} S^\dagger & \text{if } \text{wt } A = 0, \\ S^\dagger + \frac{1}{nm \text{wt } A} E & \text{if } \text{wt } A \neq 0. \end{cases}$$

Proof. By Theorem 8, $S^\dagger \in \mathcal{S}_{m,n}^o$. In the case $w := \text{wt } A \neq 0$, we find

$$\begin{aligned} (S + w E_{n,m})(S^\dagger + \frac{1}{nmw} E_{m,n})(S + w E_{n,m}) \\ = S S^\dagger S + \frac{w^2}{nmw} E_{n,m} E_{m,n} E_{n,m} = S + w E_{n,m} \end{aligned}$$

and similarly

$$\begin{aligned} (S^\dagger + \frac{1}{nmw} E_{m,n})(S + w E_{n,m})(S^\dagger + \frac{1}{nmw} E_{m,n}) \\ = S^\dagger S S^\dagger + \frac{w}{n^2 m^2 w^2} E_{m,n} E_{n,m} E_{m,n} = S^\dagger + \frac{1}{nmw} E_{m,n}, \end{aligned}$$

bearing in mind that the product of any matrix in $\mathcal{S}_{n,m}^o$ with $E_{n,m}$ vanishes. Also, the matrices

$$(S + w E_{n,m})(S^\dagger + \frac{1}{nmw} E_{m,n}) = S S^\dagger + \frac{1}{n} E_n$$

and

$$(S^\dagger + \frac{1}{nmw} E_{m,n})(S + w E_{n,m}) = S^\dagger S + \frac{1}{m} E_m$$

are symmetric because $S S^\dagger$ and $S^\dagger S$ are. \square

In the case of a square matrix in \mathcal{S}_n represented as a sum of squares of co-Latin matrices arising from the singular value decomposition as in Theorem 5, we obtain the following formula for the pseudoinverse.

Corollary 4. *Let $A \in \mathcal{S}_n^o$ and let $C_j = a_j 1_n^* + 1_n b_j^*$, for $j \in \{1, \dots, r\}$ be co-Latin matrices such that*

$$A = \sum_{j=1}^r C_j^2 - \frac{\text{tr } A}{n} E_n$$

and such that $a_j, b_j \in \{1_n\}^\perp$ have the property that the a_j are pairwise orthogonal and the b_j are pairwise orthogonal. Then

$$A^\dagger = \sum_{j=1}^r \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j}.$$

Proof. By Lemma 2,

$$C_j^2 = n a_j b_j^* + b_j^* a_j E_n \quad (j \in \{1, \dots, r\}).$$

The matrix $A = \sum_{j=1}^r n a_j b_j^* \in \mathcal{S}_n^o$ has pseudoinverse $\sum_{j=1}^r \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j}$; indeed,

$$\begin{aligned} \sum_{j=1}^r n a_j b_j^* \sum_{k=1}^r \frac{b_k a_k^*}{n a_k^* a_k b_k^* b_k} \sum_{l=1}^r n a_l b_l^* &= \sum_{j,k,l=1}^r n a_j \frac{b_j^* b_k a_k^* a_l}{a_k^* a_k b_k^* b_k} b_l^* \\ &= \sum_{j=1}^r n a_j b_j^* \end{aligned}$$

since $a_k^* a_l = a_k^* a_k \delta_{k,l}$ and $b_j^* b_k = b_k^* b_k \delta_{j,k}$. Similarly

$$\begin{aligned} \sum_{j=1}^r \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j} \sum_{k=1}^r n a_k b_k^* \sum_{l=1}^r \frac{b_l a_l^*}{n a_l^* a_l b_l^* b_l} &= \sum_{j,k,l=1}^r \frac{b_j a_j^* a_k b_k^* b_l a_l^*}{n a_j^* a_j b_j^* b_j a_l^* a_l b_l^* b_l} \\ &= \sum_{j=1}^r \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j}. \end{aligned}$$

Moreover, the matrices

$$\sum_{j=1}^r n a_j b_j^* \sum_{k=1}^r \frac{b_k a_k^*}{n a_k^* a_k b_k^* b_k} = \sum_{j=1}^r \frac{a_j a_j^*}{a_j^* a_j}$$

and

$$\sum_{j=1}^r \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j} \sum_{k=1}^r n a_k b_k^* = \sum_{j=1}^r \frac{b_j b_j^*}{b_j^* b_j}$$

are evidently symmetric. \square

Example 5. As an example we apply the above theory to the constant sum part S_W of the Wilson matrix, considered in Example 2 (see eq (3.3)). Then, to 5 significant figures,

$$a_1 = \begin{pmatrix} -0.41387 \\ -0.55390 \\ 0.32015 \\ 0.64762 \end{pmatrix}, a_2 = \begin{pmatrix} -0.045719 \\ 0.25270 \\ -0.77900 \\ 0.57202 \end{pmatrix}, a_3 = \begin{pmatrix} 0.75936 \\ -0.61590 \\ -0.20164 \\ 0.058178 \end{pmatrix},$$

and $b_j = a_j/4$ ($j \in \{1, 2, 3\}$). Applying the construction of Corollary 4, we obtain

$$S_W^\dagger = \sum_{j=1}^3 \frac{b_j a_j^*}{n a_j^* a_j b_j^* b_j} = \begin{pmatrix} \frac{4}{3} & -1 & -\frac{1}{3} & 0 \\ -1 & 1 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{5}{6} & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

6. Decomposition of matrices and their pseudoinverses

In this section we consider the relationship between the decompositions according to Theorem 2 of a given $n \times m$ matrix $A = S + V + wE_{n,m}$ and of its pseudoinverse matrix $A^\dagger = S' + V' + w'E_{m,n}$. By Theorems 7 and 8, S and V will have respective weightless pseudoinverse matrices $S^\dagger \in \mathcal{S}_{n,m}^o$ and $V^\dagger \in \mathcal{V}_{n,m}$, where $S' \neq S^\dagger$ and $V' \neq V^\dagger$ in general. We also note that the weights w and w' are not directly related and in particular don't need to vanish together, cf. Lemma 5 below.

We first consider the general case and then give a more detailed, comprehensive set of relations between the parts of the decomposition in the special case of a regular square matrix. The calculations are simplified by the following observation.

Lemma 3. *Let $S \in \mathcal{S}_{m,n}^o$ and $V = a1_m^T + 1_n b^* \in \mathcal{V}_{n,m}$, with $n, m \in \mathbb{N}$. Then we have the following triple matrix product relations.*

1. $VE_{m,n}V = nmab^*$,
2. $E_{m,n}VE_{m,n} = SE_{n,m} = E_{n,m}S = SCS = 0$, and
3. $VSV = b^*SaE_{n,m}$.

6.1. General formulae

Rewriting the triple product identity $AA^\dagger A = A$ as

$$(S + V + wE_{n,m})(S' + V' + w'E_{m,n})(S + V + wE_{n,m}) = S + V + wE_{n,m},$$

the product on the left has 27 terms, of which 12 vanish by Lemma 3. The remaining terms give

$$\begin{aligned}
 S + V + wE_{n,m} &= SS'S + w'VE_{m,n}V + VV'S + SV'V + VV'V + SS'V + VS'S \\
 &\quad + w(SV'E_{n,m} + E_{n,m}V'S) + ww'(VE_{m,n}E_{n,m} + E_{n,m}E_{m,n}V) \\
 &\quad + w(VV'E_{n,m} + E_{n,m}V'V) + VS'V + w^2w'E_{n,m}E_{m,n}E_{n,m}.
 \end{aligned}$$

Setting $V = a1_m^T + 1_nb^*$ and $V' = a'1_n^T + 1_mb'^*$ we may rewrite this as

$$\begin{aligned}
 S + V + wE_{n,m} &= SS'S + w'nmab^* + n(Sa')b^* + mab'^*S \\
 &\quad + VV'V + 1_nb^*SS' + SS'a1_m^T + w(nSa'a1_m^T + m1_nb'^*S) + ww'nmV \\
 &\quad + w(nb^*a' + mb'^*a)E_{n,m} + (b^*S'a)E_{n,m} + nmw^2w'E_{n,m},
 \end{aligned}$$

which gives rise to three separate equations using the direct sum decomposition of the matrix space into $\mathcal{S}_{n,m}^o$, $\mathcal{V}_{n,m}$ and $\mathbb{C}E_{n,m}$.

Applying the same approach to the symmetry condition $AA^\dagger = (AA^\dagger)^*$, we obtain the following theorem; its last statement follows from the fact that A is the pseudoinverse of A^\dagger .

Theorem 10. *Let A be an $n \times m$ matrix with decomposition $A = S + V + wE_{n,m}$ and pseudoinverse matrix $A^\dagger = S' + V' + w'E_{m,n}$. Then the following identities hold,*

$$\begin{aligned}
 S &= SS'S + w'n^2ab^* + n(Sa')b^* + mab'^*S, \\
 V &= VV'V + 1_nb^*SS' + SS'a1_m^T + w(nSa'a1_m^T + m1_nb'^*S) + ww'nmV, \\
 w(1 - nb^*a' + mb'^*a - nmww') &= b^*S'a, \\
 SS' + VV' &= (SS' + VV')^*,
 \end{aligned}$$

and

$$SV' + VS' + wE_{n,m}V' + w'VE_{m,n} = (SV' + VS' + wE_{n,m}V' + w'VE_{m,n})^*.$$

These identities remain true when A, S, V, w, a and b are swapped with $A^\dagger, S', V', w', a'$ and b' .

6.2. Invertible matrices

We now relate the decomposition of an invertible matrix into its weightless constant sum, co-Latin and weight parts to the decomposition of its inverse.

It turns out that the Moore-Penrose pseudoinverse of the weightless constant sum part plays a pivotal role in this connection.

Lemma 4. *Let M be an invertible $n \times n$ matrix with inverse M^{-1} , and let $M = C + S + wE_n$ and $M^{-1} = C' + S' + w'E_n$ be their decompositions as in Theorem 2, with*

$w := \text{wt } M, w' := \text{wt } M^{-1}$. Let $C = a1^T + 1b^*, C' = a'1^T + 1b'^*$ with $a, b, a', b' \in \{1_n\}^\perp$ as in Theorem 1.

a) Then

$$b^*a' = b'^*a = \frac{1}{n} - ww'n, \tag{6.1}$$

$$wnb'^* = -b^*S', \tag{6.2}$$

$$w'nb^* = -b'^*S, \tag{6.3}$$

$$w'na = -Sa', \tag{6.4}$$

$$wna' = -S'a. \tag{6.5}$$

Moreover,

$$I_n - \frac{1}{n} E_n = nab'^* + SS' = na'b'^* + S'S. \tag{6.6}$$

b) If $w' \neq 0$, then S has rank $n - 1$ and

$$S' = S^\dagger + \frac{a'b'^*}{w'}. \tag{6.7}$$

c) If $w' = 0$, then S has rank $n - 2$.

Remark. Equations (6.2), (6.3), (6.4) and (6.5) are equivalent to the identities

$$CS' = -wE_nC', C'S = -w'E_nC, SC' = -w'CE_n \text{ and } S'C = -wC'E_n,$$

respectively.

Proof. a) We start from the equations

$$I_n = MM^{-1} = CC' + CS' + w'CE_n + SC' + SS' + wE_nC' + ww'nE_n \tag{6.8}$$

and

$$I_n = M^{-1}M = C'C + C'S + wC'E_n + S'C + S'S + w'E_nC + ww'nE_n. \tag{6.9}$$

Multiplication of equation (6.8) by E_n on the right gives

$$\begin{aligned} E_n &= CC'E_n + CS'E_n + w'nCE_n + SC'E_n + SS'E_n + wE_nC'E_n + ww'n^2E_n \\ &= n(b^*a')E_n + 0 + n1_nb^*S' + wn^21_nb'^* + 0 + 0 + ww'n^2E_n, \end{aligned}$$

so using the uniqueness of the decomposition in Theorem 2, we obtain the identities

$$1 = nb^*a' + ww'n^2, \quad 0 = n1_n(b^*S' + nwb'^*).$$

The analogous treatment of equation (6.9) gives

$$1 = nb'a + ww'n^2, \quad 0 = n1_n(b'^*S + nwb'^*).$$

These identities imply equations (6.1), (6.2) and (6.3). Furthermore, multiplying equation (6.8) by E_n on the left, we find

$$\begin{aligned} E_n &= E_nCC' + E_nCS' + w'E_nCE_n + E_nSC' + E_nSS' + wnE_nC' + ww'n^2E_n \\ &= n(b^*a')E_n + w'n^2a1_n^T + 0 + 0 + 0 + nSa'1_n^T + ww'n^2E_n, \end{aligned}$$

so the uniqueness of the decomposition of Theorem 2 gives

$$0 = (w'na + Sa')n1_n^T$$

and hence equation (6.4). An analogous calculation starting from equation (6.9) yields equation (6.5). The identities (6.6) follow by using equations (6.1), (6.2) and (6.4) in equation (6.8) and by using equation (6.1), (6.3) and (6.5) in equation (6.9), respectively.

b) We can use equation (6.4) to rewrite equation (6.6) in the form

$$I_n - \frac{1}{n}E_n = -\frac{1}{w'}Sa'b'^* + SS' = S\left(-\frac{a'b'^*}{w'} + S'\right),$$

which implies that S has rank $n - 1$ (note that this is the maximal possible rank for a weightless constant sum matrix). In particular, both the range of S and the orthogonal complement of the null space of S are equal to $\{1_n\}^\perp$. For the Moore-Penrose pseudoinverse S^\dagger , this means that $SS^\dagger = S^\dagger S = I_n - \frac{1}{n}E_n$. Hence the above identity yields

$$\begin{aligned} S^\dagger &= S^\dagger SS^\dagger = S^\dagger\left(I_n + \frac{1}{n}E_n\right) = S^\dagger S\left(S' - \frac{a'b'^*}{w'}\right) \\ &= \left(I_n - \frac{1}{n}E_n\right)\left(S' - \frac{a'b'^*}{w'}\right) = S' - \frac{a'b'^*}{w'}. \end{aligned}$$

c) From $M = a1_n^T + 1_nb^* + S + w1_n1_n^T$ it is evident that $\text{ran } M = \text{ran } S + \text{span}\{1_n, a\}$, where $\text{ran } A$ denotes the range $\{Ax \mid x \in \mathbb{C}^n\}$ of an $n \times n$ matrix A . As M has full rank, it follows that S has rank at least $n - 2$. If $w' = 0$, then by equation (6.4) $Sa' = 0$. Now $a' \neq 0$ since otherwise equation (6.1) gives the contradiction $0 = \frac{1}{n}$. Hence the null space of S contains the two non-null orthogonal vectors a' and 1_n . \square

We next note that the weight of the inverse matrix M^{-1} is determined by the determinants of M and of $M + E_n$; interestingly, it has no connection with the weight of M itself.

Lemma 5. *Let M be an invertible $n \times n$ matrix. Then the weight of its inverse is*

$$\text{wt } M^{-1} = \frac{\det(M + E_n) - \det M}{n^2 \det M}. \tag{6.10}$$

Proof. Writing the inverse in terms of the adjugate matrix [5], $M^{-1} = \frac{1}{\det M} \text{adj } M$, Lemma 4.1 of [8] with $u = v = 1_n$ gives

$$\det(M + E_n) = \det M + 1_n^T (\text{adj } M) 1_n = \det M + n^2 \text{wt}(M^{-1} \det M),$$

and the claimed identity follows by rearrangement, using the linearity of the weight function. \square

Remark. Equation (6.10) shows that the weight of the inverse matrix vanishes if and only if $\det(M + E_n) = \det M$. By a scaling argument, this can be seen to be equivalent to $\det(M + \alpha E_n) = \det M$ for all non-zero numbers α . However, differentiation with respect to α gives nothing new, as $\frac{d}{d\alpha} \det(M + \alpha E_n) |_{\alpha=0} = n^2 \text{wt}(\text{adj } M)$.

In the following theorem, we show that, once its weight has been obtained by equation (6.10), the components of the inverse matrix can be found in terms of the co-Latin part of M and the pseudoinverse of its weightless constant sum matrix part, provided both weights do not vanish; together with equation (6.10), this gives a description of the non-linearity involved in taking the inverse.

Theorem 11. *Let M be an invertible $n \times n$ matrix with inverse M^{-1} , and let $M = C + S + w E_n$ and $M^{-1} = C' + S' + w' E_n$ be their decompositions as in Theorem 2, with $w := \text{wt } M$, $w' := \text{wt } M^{-1}$. Let $C = a 1^T + 1 b^*$, $C' = a' 1^T + 1 b'^*$ with $a, b, a', b' \in \{1_n\}^\perp$ as in Theorem 1. Assume that $w, w' \neq 0$; then*

$$\begin{aligned} C' &= -nw'(S^\dagger C + CS^\dagger), \\ S' &= S^\dagger + w' S^\dagger C E_n C S^\dagger. \end{aligned}$$

Proof. Using equations (6.2), (6.5) and (6.7),

$$\begin{aligned} C' &= a' 1_n^T + 1_n b'^* = -\frac{1}{nw} S' a 1_n^T - \frac{1}{nw} 1_n b^* S' = -\frac{1}{wn} (S' C + C S') \\ &= -\frac{1}{wn} (S^\dagger C + \frac{a' b'^*}{w'} C + C \frac{a' b'^*}{w'} + C S^\dagger) \\ &= -\frac{1}{wn} (S^\dagger C + C S^\dagger + \frac{a' 1_n^T}{w'} (b'^* a) + (b^* a') \frac{1_n b'^*}{w'}) \\ &= -\frac{1}{wn} (S^\dagger C + C S^\dagger + \frac{1}{w'} (\frac{1}{n} - w w' n) C') \\ &= -\frac{1}{wn} (S^\dagger C + C S^\dagger) + C' - \frac{1}{w w' n^2} C', \end{aligned}$$

and the claimed formula for C' follows by rearrangement. Furthermore, equation (6.7) gives

$$\begin{aligned} S' &= S^\dagger + \frac{a'b'^*}{w'} = S^\dagger + \frac{1}{w'n^2} C' E_n C' \\ &= S^\dagger + \frac{n^2 w'^2}{w'n^2} (S^\dagger C + C S^\dagger) E_n (S^\dagger C + C S^\dagger) \\ &= S^\dagger + w' S^\dagger C E_n C S^\dagger, \end{aligned}$$

noting that S^\dagger is again a weightless constant sum matrix by Theorem 8. \square

Example 6. For the Wilson matrix the construction of Theorem 11 gives us $C' = -nw'(S^\dagger C + C S^\dagger)$

$$\begin{aligned} &= -4 \times \frac{3}{8} \left(\frac{1}{12} \begin{pmatrix} -37 & -37 & -37 & -37 \\ 27 & 27 & 27 & 27 \\ 13 & 13 & 13 & 13 \\ -3 & -3 & -3 & -3 \end{pmatrix} + \frac{1}{12} \begin{pmatrix} -37 & 27 & 13 & -3 \\ -37 & 27 & 13 & -3 \\ -37 & 27 & 13 & -3 \\ -37 & 27 & 13 & -3 \end{pmatrix} \right) \\ &= \frac{1}{4} \begin{pmatrix} 37 & 5 & 12 & 20 \\ 5 & -27 & -20 & -12 \\ 12 & -20 & -13 & -5 \\ 20 & -12 & -5 & 3 \end{pmatrix} \end{aligned}$$

and $S' = S^\dagger + w' S^\dagger C E_n C S^\dagger$

$$\begin{aligned} &= \frac{1}{6} \begin{pmatrix} 8 & -6 & -2 & 0 \\ -6 & 6 & 0 & 0 \\ -2 & 0 & 5 & -3 \\ 0 & 0 & -3 & 3 \end{pmatrix} + \frac{3}{8} \times \frac{1}{9} \begin{pmatrix} 1369 & -999 & -481 & 111 \\ -999 & 729 & 351 & -81 \\ -481 & 351 & 169 & -39 \\ 111 & -81 & -39 & 9 \end{pmatrix} \\ &= \frac{1}{24} \begin{pmatrix} 1369 & -999 & -481 & 111 \\ -999 & 729 & 351 & -81 \\ -481 & 351 & 169 & -39 \\ 111 & -81 & -39 & 9 \end{pmatrix}. \end{aligned}$$

Remark 5. Theorem 11 offers an alternative way of representing the inverse of an invertible matrix, based on the symmetry type decomposition shown in Section 2. This suggests a possible area for further investigation applying our results, as it may be possible to obtain the inverses of ill-conditioned matrices more readily in terms of less ill-conditioned matrices. The formulae in Theorem 11 only require (after the decomposition of the matrix M) finding the pseudoinverse of the constant-sum part S and the weight w' of the inverse matrix, which, along with the weight of M , must be non-zero for the formulae to be valid. The matrix S^\dagger is a pseudoinverse, but in the situation where the rank of S

equals $n-1$ — which, by Lemma 4 b) and c) is equivalent to $w' \neq 0$ and can thus be used to ascertain this without calculating w' —, its null space and co-kernel are known to be equal to $\{1_n\}^\perp$, so the pseudoinverse can be calculated as the inverse of an invertible $(n-1) \times (n-1)$ matrix. Calculation of w' by equation (6.10) requires calculation of two determinants and may therefore not be numerically efficient for matrices of large size; however, w' can be obtained more directly once S^\dagger and the fact that $w' \neq 0$ are known. Indeed, by Theorem 11 $M^{-1} = S^\dagger + w'(S^\dagger C E_n C S^\dagger - n(S^\dagger C + C S^\dagger))$, so

$$1_n = M M^{-1} 1_n = w' M (n 1_n - n^2 S^\dagger a),$$

which determines w' .

For the Wilson matrix, we find that the eigenvalues of S are 3.95536, 0.846797, 0.447843 and 0, so the ratio of the largest and smallest non-zero eigenvalues is equal to 8.83202, which is considerably less than the condition number of W , $\kappa_2(W) \approx 3 \times 10^3$.

Declaration of competing interest

The authors declare that they have no known competing interests.

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No data was used for the research described in the article.

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