Cholesky factorization of almost all non-positive matrices

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Positive definite matrices

A real symmetric matrix $A \in \mathbb{R}^{n \times n}$ is *positive definite* ($A \in PD_n$) if any of the following holds:

1. $\mathbf{u}^T A \mathbf{u} > 0$ for all $\mathbf{0} \neq \mathbf{u} \in \mathbb{R}^n$.
2. The eigenvalues of A are all in $(0, \infty)$.
3. $A = B^T B$ for some invertible $B \in \mathbb{R}^{n \times n}$.
4. There exists a basis of $\mathbb{R}^n$, say $\mathbf{x}_1, \dots, \mathbf{x}_n$, such that A is its Gram matrix: $a_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$ for all $1 \leqslant i, j \leqslant n$.
5. The principal minor $\det A_{I \times I}$ is positive, for all $I \subseteq [n] := \{1, \dots, n\}$.

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5. The principal minor $\det A_{I \times I}$ is positive, for all $I \subseteq [n] := \{1, \dots, n\}$.
6. The *Leading Principal Minor (LPM)* $\det A_{[k] \times [k]} > 0$ for all $1 \leqslant k \leqslant n$.

We will weaken this condition, and study the larger matrix class.

The Cholesky factorization

One hundred years ago, the following fundamental fact appeared:

Theorem (Cholesky, in Benoit's publication, 1924)

For any positive definite matrix A, there exists a unique matrix L satisfying:

1. *L is real and lower triangular.*
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Definition

This is called the Cholesky factorization of A. *Let* ***Cholesky space*** $\mathbf{L}_n$ *consist of all L satisfying (1) and (2) above.*

Cholesky decomposition: widely used in numerical analysis, statistics, and downstream applications. E.g., it is of interest to Cholesky-factor *covariance matrices* – these are Gram matrices of vectors in Euclidean space.

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What about decomposing symmetric matrices with negative eigenvalues?

1. LPM cones and generalized Cholesky factorization

LDU decomposition

For *generic* real (symmetric) matrices, one has the *LDU decomposition*.

Definition

Given $n \geqslant 1$, *denote by* LPM_n *the cone of symmetric matrices in* $\mathbb{R}^{n\times n}$ *with nonzero Leading Principal Minors.*

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Every LPM_n matrix can be uniquely decomposed into $L_1 D L_1^T$, where L_1 is lower triangular with all diagonal entries 1, and D is diagonal.

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Is there a generalization of the Cholesky decomposition, e.g. to LPM_n – which specializes to the Cholesky on positive definite matrices?

Studying the LPM cone: I

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$$a_{11} = +, \quad \det(A) = +, \qquad a_{11} = -, \quad \det(A) = +$$
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In general?

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- a_{11} is positive or negative,
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Collect together $\epsilon = (\epsilon_1, \dots, \epsilon_n) \in \{-1, 1\}^n$, where $\epsilon_k =$ sign of $k \times k$ LPM.

Definition

Given a sign pattern $\epsilon \in \{-1, 1\}^n$, *define*
$LPM_n(\epsilon) := \{$ *all real symmetric* $A_{n \times n}$ *with* $\operatorname{sgn}(\det A_{[k] \times [k]}) = \epsilon_k$ *for all* $k\,\}$.

Studying the LPM cone: II

$$LPM_n(\epsilon) := \{A \text{ real symmetric } : \operatorname{sgn}(\det A_{[k]\times[k]}) = \epsilon_k \ \forall k\}.$$

Examples of $LPM_n(\epsilon)$:

- If all $\epsilon_k = 1$, then $LPM_n(\mathbf{1}_n) = PD_n$ – positive definite matrices.
- What is the ϵ for negative definite matrices?

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  Then $-A \in PD_n$, so $\det A_{[k]\times[k]}$ has sign $(-1)^k$.

Proposition

1. *The cone LPM_n is a disjoint union / can be partitioned:*
   $LPM_n = \bigsqcup_{\epsilon \in \{-1,1\}^n} LPM_n(\epsilon)$.

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2. *LPM_n is open and dense in all real symmetric matrices.*
3. *The complement of LPM_n in symmetric matrices has zero Lebesgue measure.*

Extending the Cholesky decomposition to the LPM cone

Every $LPM_n(\epsilon)$ has a unique diagonal matrix with entries ± 1:

$$\mathbb{D}_\epsilon := \begin{pmatrix} \epsilon_0\epsilon_1 & 0 & 0 & \cdots & 0 \\ 0 & \epsilon_1\epsilon_2 & 0 & \cdots & 0 \\ 0 & 0 & \epsilon_2\epsilon_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \epsilon_{n-1}\epsilon_n \end{pmatrix}, \qquad \text{where } \epsilon_0 := 1.$$

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E.g. for $\epsilon = \mathbf{1}_n$, the cone $LPM_n(\mathbf{1}_n) = PD_n$ contains $\mathbb{D}_{\mathbf{1}} = \mathrm{Id}_n$.

Question: An "LDU-alternative" is $L\mathbb{D}_\epsilon L^T$. Is this in $LPM_n(\epsilon)$ for all ϵ?
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Theorem (K.–Vishwakarma, 2025)

Let $n \geqslant 1$ and $\epsilon \in \{-1,1\}^n$. For every matrix $A \in LPM_n(\epsilon)$, there exists a unique $L \in \mathbf{L}_n$ such that $A = L\mathbb{D}_\epsilon L^T$.

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$$\Phi_{\mathbb{D}_\epsilon} : \mathbf{L}_n \to LPM_n(\epsilon); \qquad L \mapsto L\mathbb{D}_\epsilon L^T.$$

(The usual Cholesky decomposition is $\Phi_{\mathbb{D}_{\mathbf{1}}}^{-1}$.)

Cholesky-factoring all symmetric matrices?

Fact: The Cholesky decomposition for PD_n extends to *all psd matrices* $\overline{PD_n}$.

What about other cones? E.g., perturb – factorize – take limit?

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(First) difference between PD and other LPM cones:

If A is positive semidefinite (but not pd),
and $A_k = (A + \frac{1}{k}\mathrm{Id}) = L_k L_k^T$ is "usual" Cholesky-factored,
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Reason: In the C^*-algebra $\mathcal{B}(\mathbb{R}^n)$,

$$\|A_k\| = \|L_k L_k^T\| = \|L_k\|^2.$$

Not true in other LPM cones.

Cholesky decomposition is algorithmic

Further properties of $\Phi_{\mathbb{D}_\epsilon}$?

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Theorem (K.–Vishwakarma, 2025)

*For all $n \geqslant 1$ and $\epsilon \in \{-1, 1\}^n$, the map $\Phi_{\mathbb{D}_\epsilon}^{-1}$ is an **algorithmic** smooth diffeomorphism : $LPM_n(\epsilon) \to \mathbf{L}_n$.*

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Moreover, the smooth diffeos $\Phi_{\mathbb{D}_\epsilon}^{\pm 1}$ preserve the Borel and Lebesgue sets.

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Moreover, the smooth diffeos $\Phi_{\mathbb{D}_\epsilon}^{\pm 1}$ preserve the Borel and Lebesgue sets.

- See our preprint for the algorithm.
- As a result, "good" structures on Cholesky space $\mathbf{L}_n$ (of lower triangular matrices with positive diagonals) transfer to every $LPM_n(\epsilon)$.
- We will explore several such structures: Riemannian manifolds, abelian Lie groups, and more.

2. Riemannian manifold structure(s); Lie group

Riemannian metric on the PD cone

Another difference between the PD cone and other LPM cones:

The PD cone is a Riemannian manifold (Bhatia–Holbrook, ...):

$$d(A,B) := \| \log(\lambda_1), \dots, \log(\lambda_n) \|,$$

where λ_j are the (positive!) eigenvalues of AB^{-1} – or of $B^{-1/2}AB^{-1/2}$.

Question: What about other LPM cones?

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Question: What about other LPM cones? Not clear.

Recently, an alternative Riemannian structure was proposed – not on PD_n, but on Cholesky space $\mathbf{L}_n$!

Riemannian metric on Cholesky space

Theorem (Lin, SIMAX 2019)

The space $\mathbf{L}_n$ is a Riemannian manifold, with the following properties:

1. *The **tangent space** at each $L \in \mathbf{L}_n$ is the lower triangular flat space $\mathbb{R}^{n(n+1)/2}$.*
2. *For tangent vectors X, Y at $L \in \mathbf{L}_n$, the **Riemannian metric** is*
$$\widetilde{g}_L(X,Y) = \sum_{i>j} x_{ij} y_{ij} + \sum_{j=1}^{n} x_{jj} y_{jj} l_{jj}^{-2}.$$
3. *The **Riemannian distance** between $L = (l_{ij})$ and $K = (k_{ij})$ in $\mathbf{L}_n$ is*
$$d_{\mathbf{L}_n}(L,K) = \left(\sum_{i>j} (l_{ij} - k_{ij})^2 + \sum_{j=1}^{n} (\log l_{jj} - \log k_{jj})^2 \right)^{1/2}.$$

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Corollary: These structures transfer to every cone $LPM_n(\epsilon)$, via the diffeomorphism $\Phi_{\mathbb{D}_\epsilon}$.

Abelian Lie group structure

Given a square matrix A, define $\mathbb{D}(A)$ to be $\operatorname{diag}(a_{11}, \ldots, a_{nn}) = A \circ \mathrm{Id}_n$.
Now define $\lfloor A \rfloor := A - \mathbb{D}(A)$.

Theorem (Lin, SIMAX 2019)

Cholesky space $\mathbf{L}_n$ *is also an abelian Lie group, with identity* Id_n, *and the product and inverse given by:*

$$L \circledcirc K = \lfloor L \rfloor + \lfloor K \rfloor + \mathbb{D}(L)\mathbb{D}(K), \qquad L_{\circledcirc}^{-1} = -\lfloor L \rfloor + \mathbb{D}(L)^{-1}.$$

Moreover, the Riemannian metric is bi-invariant under this group structure.

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- Lin moreover shows that this manifold $\mathbf{L}_n$ has zero sectional curvature.
- This naturally leads to asking: is this manifold in fact flat Euclidean space ?

  Lin writes in his work: *"... the so-called Cholesky manifold in [17] is a Riemannian submanifold of a Euclidean space, while our Riemannian manifold to be proposed is not."*

Cholesky space is Euclidean space!

However, in fact $\mathbf{L}_n$ **is** Euclidean space!

Theorem (K.–Vishwakarma, 2025)

1. *Define "scalar multiplication"* $\cdot : \mathbb{R} \times \mathbf{L}_n \to \mathbf{L}_n$ *via:* $\alpha \cdot L := \alpha \lfloor L \rfloor + \mathbb{D}(L)^\alpha$. *Then the map*

$$\eta : (\mathbf{L}_n, \circledcirc, \cdot) \to (\mathbb{R}^{n(n+1)/2}, +, \cdot)$$

defined by $\eta(L) := (\{l_{ij} : i > j\}\,; \log l_{11}, \dots, \log l_{nn})$, *is an* $\mathbb{R}$*-vector space isomorphism.*

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defined by $\eta(L) := (\{l_{ij} : i > j\}\,;\, \log l_{11}, \ldots, \log l_{nn})$, *is an* $\mathbb{R}$*-vector space isomorphism.*
2. *Also define the form* $\langle \cdot, \cdot \rangle : \mathbf{L}_n^2 \to \mathbf{L}_n$ *defined by*
$$\langle L, K \rangle := \sum_{i>j} l_{ij} k_{ij} + \sum_{j=1}^{n} \log(l_{jj}) \log(k_{jj}).$$
Then $\langle \cdot, \cdot \rangle$ *is* $\mathbb{R}$*-bilinear,*

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Theorem (K.–Vishwakarma, 2025)

1. *Define "scalar multiplication"* $\cdot : \mathbb{R} \times \mathbf{L}_n \to \mathbf{L}_n$ *via:* $\alpha \cdot L := \alpha \lfloor L \rfloor + \mathbb{D}(L)^{\alpha}$. *Then the map*
$$\eta : (\mathbf{L}_n, \circledcirc, \cdot) \to (\mathbb{R}^{n(n+1)/2}, +, \cdot)$$
defined by $\eta(L) := (\{l_{ij} : i > j\}; \log l_{11}, \dots, \log l_{nn})$, *is an* $\mathbb{R}$*-vector space isomorphism.*
2. *Also define the form* $\langle \cdot, \cdot \rangle : \mathbf{L}_n^2 \to \mathbf{L}_n$ *defined by*
$$\langle L, K \rangle := \sum_{i>j} l_{ij} k_{ij} + \sum_{j=1}^{n} \log(l_{jj}) \log(k_{jj}).$$
Then $\langle \cdot, \cdot \rangle$ *is* $\mathbb{R}$*-bilinear, and for all* $L, K \in \mathbf{L}_n$ *we have* $d_{\mathbf{L}_n}(L, K)^2 = \langle L -' K, L -' K \rangle, \quad L -' K := L \circledcirc K_{\circledcirc}^{-1} = \eta^{-1}(\eta(L) - \eta(K))$.

So $(\mathbf{L}_n, \langle \cdot, \cdot \rangle)$ *is isometrically isomorphic to Euclidean space* $\mathbb{R}^{n(n+1)/2}$.

3. Jacobian calculations; probability densities

Are all LPM_n cones equally big?

We saw that $LPM_n = \bigsqcup_\epsilon LPM_n(\epsilon)$,
and each cone $LPM_n(\epsilon)$ is diffeomorphic to $\mathbf{L}_n$.

- Thus one can do "**change of variables**", and switch between PD_n and each $LPM_n(\epsilon)$.

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- **Question:** Are the cones "equally big"? I.e., what is (the determinant of) the Jacobian of the **transfer map** $\Phi_{\mathbb{D}_\epsilon} \circ \Phi_{\mathbb{D}_\mathbf{1}}^{-1} : PD_n \to LPM_n(\epsilon)$?
  Is its modulus 1?

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Theorem (K.–Vishwakarma, 2025)

Set $\epsilon_0 := 1$. The Jacobian of $\Phi_{\mathbb{D}_\epsilon}$ at any $L \in \mathbf{L}_n$ is lower triangular in the lexicographic order, and its determinant equals

$$\det \left(\frac{\partial \Phi_{\mathbb{D}_\epsilon}(L)_{ij}}{\partial l_{i'j'}} \right)_{\substack{1 \leqslant j \leqslant i \leqslant n \\ 1 \leqslant j' \leqslant i' \leqslant n}} = 2^n \prod_{j=1}^n (l_{jj} \epsilon_{j-1} \epsilon_j)^{n+1-j}.$$

Hence the Jacobian-determinant of $\Phi_{\mathbb{D}_\epsilon} \circ \Phi_{\mathbb{D}_\mathbf{1}}^{-1}$ is ± 1.

Consequences of Jacobian calculations

- Firstly: yes, for any n all cones $LPM_n(\epsilon)$ are "equally big"! So, we have extended the Cholesky factorization on PD_n to all of LPM_n, which is 2^n times "as big".

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- Firstly: yes, for any n all cones $LPM_n(\epsilon)$ are "equally big"! So, we have extended the Cholesky factorization on PD_n to all of LPM_n, which is 2^n times "as big".
- Second: the "transfer maps" $\Phi_{\mathbb{D}_\epsilon} \circ \Phi_{\mathbb{D}_{\mathbf{1}}}^{-1}$ are all Lebesgue measure-preserving smooth diffeomorphisms.

Corollary (K.–Vishwakarma, 2025)

Fix $n \geqslant 1$, and let μ be any probability density that

1. *is absolutely continuous w.r.t. Lebesgue measure, and*
2. *has equal mass on each $LPM_n(\epsilon)$ cone.*

Then the Cholesky algorithm fails with probability $1 - 2^{-n}$, but our "generalized Cholesky decomposition" works w.p. 1.

Algorithm to detect ϵ and L?

Our generalized Cholesky decomposition is "nice" algorithmically too – one can adopt usual Cholesky algorithms to detect ϵ too.

E.g.: adapt the Cholesky–Banachiewicz and Cholesky–Crout algorithms to compute the decomposition "fast":

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LPM-Cholesky factorization: obtaining ϵ and L from A:

1. **Input:** integer $n \geqslant 1$ and matrix $A \in LPM_n^{\mathbb{C}}$, to be Cholesky-factored.
2. Set $\epsilon_0 := 1$.
3. For $j = 1, \dots, n$:
    - $\epsilon_j := \operatorname{sign}\left(\epsilon_{j-1}\left(a_{jj} - \sum_{i=1}^{j-1} \epsilon_{i-1}\epsilon_i |l_{ji}|^2\right)\right)$.
    - $l_{jj} := \sqrt{\epsilon_{j-1}\epsilon_j \left(a_{jj} - \sum_{i=1}^{j-1} \epsilon_{i-1}\epsilon_i |l_{ji}|^2\right)}$.
    - For $k = j+1, \dots, n$:
        - $l_{jk} = 0$.
        - $l_{kj} = \frac{\epsilon_{j-1}\epsilon_j}{l_{jj}} \left(a_{kj} - \sum_{i=1}^{j-1} \epsilon_{i-1}\epsilon_i l_{ki}\overline{l_{ji}}\right)$.
4. **Output/Return:** ϵ, L (such that $A = L\mathbb{D}_\epsilon L^T$).

Additional consequences of Jacobian calculations

- One can do multivariate analysis/integration on every cone $LPM_n(\epsilon)$ by reducing to the PD-cone! (Recall that $\Phi_{\mathbb{D}_\epsilon}^{\pm 1}$ preserved Borel/Lebesgue sets, and hence their σ-algebras.)

Additional consequences of Jacobian calculations

- One can do multivariate analysis/integration on every cone $LPM_n(\epsilon)$ by reducing to the PD-cone! (Recall that $\Phi_{\mathbb{D}_\epsilon}^{\pm 1}$ preserved Borel/Lebesgue sets, and hence their σ-algebras.)
- This also allows us to "transfer" *probability densities* – like the Wishart distribution – from PD_n to every cone $LPM_n(\epsilon)$. In particular, by "averaging" we obtain probability distributions supported on the entire open dense cone LPM_n.
- Thus, the Cholesky decompositions / transfer maps $\Phi_{\mathbb{D}_\epsilon} \circ \Phi_{\mathbb{D}_{\mathbf{1}}}^{-1}$ naturally lead to random matrix theory on LPM-cones.

4. Other remarks

TPM matrices – trailing principal minors

Yet another characterization of $A = A^T$ being positive definite:

*If and only if the **trailing** principal minors are all* > 0.

Thus – **define**
$TPM_n(\epsilon) := \{$ all real symmetric $A_{n \times n}$ with kth TPM of sign $\epsilon_k, \forall k \}$.

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This approach proceeds completely parallel to the LPM results – everything goes through "as expected" – because of a linear transition map:

Theorem (K.–Vishwakarma, 2025)

Let P_n be the anti-diagonal $n \times n$ permutation matrix.
For all $n \geqslant 1$, the map $\Phi(M) := (P_n M P_n)^T$ is a linear (smooth) diffeomorphism : $\mathbf{L}_n \to \mathbf{L}_n$,

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This yields a *UDL*-type factorization of "almost all" symmetric matrices. Once again, this is not the same as the one in the literature, but generalizes the Cholesky decomposition instead.

Inertia of LPM matrices

By Sylvester's law and the Cholesky-type factorization $\Phi_{\mathbb{D}_\epsilon}^{-1}$, every matrix in $LPM_n(\epsilon)$ has the same inertia as $\mathbb{D}_\epsilon$. What is its inertia?

- Equivalently, how many negative eigenvalues does it have?
- For $0 \leqslant k \leqslant n$, for how many ϵ does $\mathbb{D}_\epsilon$ have exactly k negative eigenvalues?

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Theorem (K.–Vishwakarma, 2025)

1. *For $n \geqslant 1$ and $\epsilon \in \{-1, 1\}^n$, the diagonal matrix $\mathbb{D}_\epsilon$ has precisely $\vartheta(1; \epsilon)$ negative eigenvalues. Here, $\vartheta(1; \epsilon)$ denotes the number of sign changes in the sequence $\epsilon_0 = 1, \epsilon_1, \epsilon_2, \ldots, \epsilon_n$.*

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As an amusing corollary: by counting, we just showed $\binom{n}{0} + \cdots + \binom{n}{n} = 2^n$!

SSRPM matrices

What happens if we go back to the "Sylvester" definition of PD matrices?

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Generalization: Given a sign pattern $\epsilon = (\epsilon_1, \dots, \epsilon_n) \in \{\pm 1\}^n$, define an $n \times n$ real symmetric matrix to have the
SSRPM property (Strictly Sign Regular Principal Minors), if:

- **all** 1×1 principal minors (= diagonal entries) are nonzero, with sign ϵ_1;
- **all** 2×2 principal minors are nonzero, with sign ϵ_2;
- $\dots$
- **all** $n \times n$ principal minors (= determinant) is nonzero with sign ϵ_n.

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Examples:

1. If all $\epsilon_k = 1$, these are precisely the positive definite matrices (Sylvester).
2. If all $\epsilon_k = (-1)^k$, these are the negative definite matrices.
3. (What about other ϵ?)

SSRPM matrices (cont.)

What is the pressing question, in this case?

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  Answer: Yes – because $SSRPM_n(\epsilon) \subset LPM_n(\epsilon)$ for all n, ϵ!

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  Existence: Do SSRPM matrices exist for all $n \geqslant 1$ and all $\epsilon \in \{\pm 1\}^n$?

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  Answer: Known via numerical computations/search for $n \leqslant 5$.
  Open for $n \geqslant 6$.

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