Questions to understand the topic of the lecture

- Can any singular matrix be positive definite?
- Can Cholesky decomposition be performed on matrices which are not Hermitian?
- Why when testing positive definite matrices by Gaussian elimination we cannot change the order of the rows?
- Do have negative definite matrices, i.e. Hermitian $\boldsymbol{A}$, s.t. $\forall \boldsymbol{x} \neq \mathbf{0} : \boldsymbol{x}^H \boldsymbol{A} \boldsymbol{x} < 0$, always a negative determinant?

Gram matrix

Theorem: Let V be an inner space and $X = (\boldsymbol{v}_1, \dots, \boldsymbol{v}_n)$ its basis. Then the so called *Gram matrix* $\boldsymbol{A}$ defined as $a_{i,j} = \langle \boldsymbol{v}_i | \boldsymbol{v}_j \rangle$ satisfies:

$$\forall \boldsymbol{u}, \boldsymbol{w} \in V : \langle \boldsymbol{u} | \boldsymbol{w} \rangle = [\boldsymbol{w}]_X^H \boldsymbol{A}^T [\boldsymbol{u}]_X$$

Observe that when X is orthonormal then $\boldsymbol{A} = \boldsymbol{I}_n$.

Proof: Denote $[\boldsymbol{u}]_X = (\alpha_1, \dots, \alpha_n)^T$, $[\boldsymbol{w}]_X = (\beta_1, \dots, \beta_n)^T$, i.e. $\boldsymbol{u} = \sum_{i=1}^{n} \alpha_i \boldsymbol{v}_i$ and $\boldsymbol{w} = \sum_{j=1}^{n} \beta_j \boldsymbol{v}_j$. Then we get

$$\langle \boldsymbol{u} | \boldsymbol{w} \rangle = \left\langle \sum_{i=1}^{n} \alpha_i \boldsymbol{v}_i \middle| \sum_{j=1}^{n} \beta_j \boldsymbol{v}_j \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \overline{\beta_j} \langle \boldsymbol{v}_i | \boldsymbol{v}_j \rangle = [\boldsymbol{w}]_X^H \boldsymbol{A}^T [\boldsymbol{u}]_X$$

Properties of every Gram matrix:

- As $\langle \boldsymbol{v}_i | \boldsymbol{v}_j \rangle = \overline{\langle \boldsymbol{v}_j | \boldsymbol{v}_i \rangle}$, i.e. $a_{i,j} = \overline{a_{j,i}}$, the matrix is *Hermitian*
- As $\langle \boldsymbol{u} | \boldsymbol{u} \rangle > 0$ for all $\boldsymbol{u} \neq \mathbf{0}$, it also holds that $[\boldsymbol{u}]_X^H \boldsymbol{A}^T [\boldsymbol{u}]_X > 0$.

Positive definite matrices

Definition: If a Hermitian matrix $\boldsymbol{A}$ of order n satisfies $\forall \boldsymbol{x} \in \mathbb{C}^n \setminus \mathbf{0} : \boldsymbol{x}^H \boldsymbol{A} \boldsymbol{x} > 0$, then the matrix is *positive definite*.

Applications:

- Finding extremes of real function of more variables — if the (*Hessian*) matrix obtained by the second order partial derivatives is positive definitive, then it is a local minimum.
- Extension of optimization programs.

Example: $\begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ ... but how the condition could be verified for all $\boldsymbol{x} \in \mathbb{C}^2 \setminus \mathbf{0}$?

Exercise: Show that if $\boldsymbol{A}, \boldsymbol{B}$ are positive definite of the same order then $\boldsymbol{A} + \boldsymbol{B}$ and $\boldsymbol{A}^{-1}$ are also positive definite.

Characterization of positive definite matrices

Theorem: For a Hermitian matrix $\boldsymbol{A}$ the following are equivalent:

1. $\boldsymbol{A}$ is positive definite
2. $\boldsymbol{A}$ has all eigenvalues positive
3. There is a regular matrix $\boldsymbol{U}$ such that $\boldsymbol{A} = \boldsymbol{U}^H \boldsymbol{U}$

Proof: $1 \Rightarrow 2$: As $\boldsymbol{A}$ is Hermitian, it has all eigenvalues real.
Let $\boldsymbol{x}$ be a nontrivial eigenvector corresponding to an eigenvalue λ.
Then $0 < \boldsymbol{x}^H \boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}^H \boldsymbol{x} = \lambda \langle \boldsymbol{x} | \boldsymbol{x} \rangle$. As $\langle \boldsymbol{x} | \boldsymbol{x} \rangle > 0$, we get $\lambda > 0$.

$2 \Rightarrow 3$: As $\boldsymbol{A}$ is Hermitian, there are unitary $\boldsymbol{R}$ and diagonal $\boldsymbol{D}$ such that $\boldsymbol{A} = \boldsymbol{R}^H \boldsymbol{D}\boldsymbol{R}$. Set a diagonal matrix $\tilde{\boldsymbol{D}} : \tilde{d}_{ii} = \sqrt{d_{ii}}$, and $\boldsymbol{U} = \tilde{\boldsymbol{D}}\boldsymbol{R}$. Now $\boldsymbol{U}^H \boldsymbol{U} = (\tilde{\boldsymbol{D}}\boldsymbol{R})^H \tilde{\boldsymbol{D}}\boldsymbol{R} = \boldsymbol{R}^H \tilde{\boldsymbol{D}}^H \tilde{\boldsymbol{D}}\boldsymbol{R} = \boldsymbol{R}^H \boldsymbol{D}\boldsymbol{R} = \boldsymbol{A}$.
$\boldsymbol{U}$ is regular since unitary and diagonal matrices are regular too.

$3 \Rightarrow 1$: If $\boldsymbol{x} \in \mathbb{C}^n \setminus \boldsymbol{0}$, then $\boldsymbol{U}\boldsymbol{x} \neq \boldsymbol{0}$ because $\boldsymbol{U}$ is regular.
Now: $\boldsymbol{x}^H \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^H \boldsymbol{U}^H \boldsymbol{U}\boldsymbol{x} = (\boldsymbol{U}\boldsymbol{x})^H \boldsymbol{U}\boldsymbol{x} = \langle \boldsymbol{U}\boldsymbol{x} | \boldsymbol{U}\boldsymbol{x} \rangle > 0$.

Cholesky factorization

Theorem: For any positive definite matrix $\boldsymbol{A}$ there is a *unique* upper triangular matrix $\boldsymbol{U}$ with positive diagonal such that $\boldsymbol{A} = \boldsymbol{U}^H \boldsymbol{U}$. The matrix $\boldsymbol{U}$ is called the *Cholesky factorization*.

Input: A Hermitian matrix $\boldsymbol{A}$
Output: The Cholesky factorization $\boldsymbol{U}$ if $\boldsymbol{A}$ is positive definite
for $i = 1, \ldots, n$ **do**

$$u_{i,i} = \sqrt{a_{i,i} - \sum_{k=1}^{i-1} \overline{u_{k,i}} u_{k,i}}$$

if $u_{i,i} \notin \mathbb{R}^+$ **then** STOP, $\boldsymbol{A}$ is not positive definite;
for $j = i+1, \ldots, n$ **do**

$$u_{i,j} = \frac{1}{u_{i,i}} \left(a_{i,j} - \sum_{k=1}^{i-1} \overline{u_{k,i}} u_{k,j} \right)$$

end
end

Example — Cholesky factorization

For a Hermitian matrix $\boldsymbol{A}$ find a triangular matrix $\boldsymbol{U}$ satisfying: $\boldsymbol{A} = \boldsymbol{U}^H\boldsymbol{U}$

$$\begin{array}{c|c} & \boldsymbol{U} \\ \hline \boldsymbol{U}^H & \boldsymbol{A} \end{array}$$

$$\begin{array}{cccc|cccc}
 & & & & 2 & 1 & 0 & -1 \\
 & & & & 0 & 1 & 2 & 3 \\
 & & & & 0 & 0 & 1 & 1 \\
 & & & & 0 & 0 & 0 & 3 \\ \hline
2 & 0 & 0 & 0 & 4 & 2 & 0 & -2 \\
1 & 1 & 0 & 0 & 2 & 2 & 2 & 2 \\
0 & 2 & 1 & 0 & 0 & 2 & 5 & 7 \\
-1 & 3 & 1 & 3 & -2 & 2 & 7 & 20
\end{array}$$

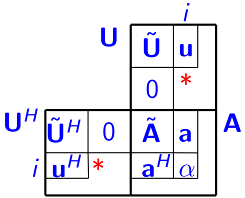
$$u_{i,i} = \sqrt{a_{i,i} - \sum_{k=1}^{i-1} \overline{u_{k,i}}\, u_{k,i}}$$

$$\begin{array}{cccc|cccc}
 & & & & 2 & 1 & 0 & -1 \\
 & & & & 0 & 1 & 2 & 3 \\
 & & & & 0 & 0 & ? & . \\
 & & & & 0 & 0 & 0 & . \\ \hline
2 & 0 & 0 & 0 & 4 & 2 & 0 & -2 \\
1 & 1 & 0 & 0 & 2 & 2 & 2 & 2 \\
0 & 2 & ? & 0 & 0 & 2 & 5 & 7 \\
-1 & 3 & . & . & -2 & 2 & 7 & 20
\end{array}$$

$$u_{i,j} = \frac{1}{u_{i,i}}\left(a_{i,j} - \sum_{k=1}^{i-1} \overline{u_{k,i}}\, u_{k,j}\right)$$

$$\begin{array}{cccc|cccc}
 & & & & 2 & 1 & 0 & -1 \\
 & & & & 0 & 1 & 2 & 3 \\
 & & & & 0 & 0 & 1 & ? \\
 & & & & 0 & 0 & 0 & . \\ \hline
2 & 0 & 0 & 0 & 4 & 2 & 0 & -2 \\
1 & 1 & 0 & 0 & 2 & 2 & 2 & 2 \\
0 & 2 & 1 & 0 & 0 & 2 & 5 & 7 \\
-1 & 3 & . & . & -2 & 2 & 7 & 20
\end{array}$$

Correctness of Cholesky factorization



Assume that the algorithm fails $*$ during the i-th iteration, i.e. $\alpha \le \boldsymbol{u}^H\boldsymbol{u}$.
We have $\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{U}}^H\tilde{\boldsymbol{U}}$ and $\boldsymbol{a} = \tilde{\boldsymbol{U}}^H\boldsymbol{u}$.

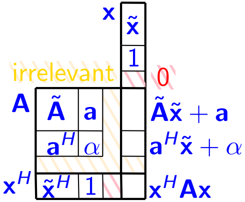
Let $\boldsymbol{x}^T = \boxed{\tilde{\boldsymbol{x}}^T \mid 1 \mid 0 \cdots 0}$ where $\tilde{\boldsymbol{x}} = -\tilde{\boldsymbol{U}}^{-1}\boldsymbol{u}$.

Now $\boldsymbol{x}^H\boldsymbol{A}\boldsymbol{x} =$

$$= \tilde{\boldsymbol{x}}^H\tilde{\boldsymbol{A}}\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{x}}^H\boldsymbol{a} + \boldsymbol{a}^H\tilde{\boldsymbol{x}} + \alpha$$

$$= (-\tilde{\boldsymbol{U}}^{-1}\boldsymbol{u})^H(\tilde{\boldsymbol{U}}^H\tilde{\boldsymbol{U}})(-\tilde{\boldsymbol{U}}^{-1}\boldsymbol{u}) + (-\tilde{\boldsymbol{U}}^{-1}\boldsymbol{u})^H(\tilde{\boldsymbol{U}}^H\boldsymbol{u}) + (\tilde{\boldsymbol{U}}^H\boldsymbol{u})^H(-\tilde{\boldsymbol{U}}^{-1}\boldsymbol{u}) + \alpha$$

$$= \boldsymbol{u}^H\boldsymbol{u} - \boldsymbol{u}^H\boldsymbol{u} - \boldsymbol{u}^H\boldsymbol{u} + \alpha = \alpha - \boldsymbol{u}^H\boldsymbol{u} \le 0$$



Hence $\boldsymbol{A}$ is not positive definite.

A recursive condition

Theorem: A block matrix $\boldsymbol{A} = \left(\begin{array}{c|c} \alpha & \boldsymbol{a}^H \\ \hline \boldsymbol{a} & \tilde{\boldsymbol{A}} \end{array}\right)$ is positive definite

if and only if $\alpha > 0$ and the matrix $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite.

Observation: The Gaussian elimination of the first column by the first row in a Hermitian matrix yields: $\left(\begin{array}{c|c} \alpha & \boldsymbol{a}^H \\ \hline \boldsymbol{a} & \tilde{\boldsymbol{A}} \end{array}\right) \sim \left(\begin{array}{c|c} \alpha & \boldsymbol{a}^H \\ \hline \boldsymbol{0} & \tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H \end{array}\right)$

Example:

$$\left(\begin{array}{c|ccc} 4 & 2 & 0 & -1 \\ \hline 2 & 2 & 2 & 2 \\ 0 & 2 & 5 & 7 \\ -1 & 2 & 7 & 20 \end{array}\right) \sim\sim \left(\begin{array}{c|ccc} 4 & 2 & 0 & -1 \\ \hline 0 & 1 & 2 & \frac{5}{2} \\ 0 & 2 & 5 & 7 \\ 0 & \frac{5}{2} & 7 & \frac{79}{4} \end{array}\right)$$

A recursive condition

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if and only if $\alpha > 0$ and the matrix $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite.

Corollary: Positive definite matrices can be recognized by Gaussian elimination, but columns should be eliminated in the top to bottom manner by subtracting appropriate multiples of the pivot rows from the rows below, i.e. the order of the rows must not change nor the rows can be multiplied by a scalar.

If the resulting upper triangular matrix has positive diagonal, then the original matrix was positive definite.

Example:

$$\left(\begin{array}{c|ccc} 4 & 2 & 0 & -1 \\ \hline 2 & 2 & 2 & 2 \\ 0 & 2 & 5 & 7 \\ -1 & 2 & 7 & 20 \end{array}\right) \sim\sim \left(\begin{array}{c|c|cc} 4 & 2 & 0 & -1 \\ \hline 0 & 1 & 2 & \frac{5}{2} \\ \cline{2-4} 0 & 2 & 5 & 7 \\ 0 & \frac{5}{2} & 7 & \frac{79}{4} \end{array}\right) \sim\sim \left(\begin{array}{c|c|c|c} 4 & 2 & 0 & -1 \\ \hline 0 & 1 & 2 & \frac{5}{2} \\ \cline{2-4} 0 & 0 & 1 & 2 \\ \cline{3-4} 0 & 0 & 2 & \frac{27}{2} \end{array}\right) \sim\sim \left(\begin{array}{c|c|c|c} 4 & 2 & 0 & -1 \\ \hline 0 & 1 & 2 & \frac{5}{2} \\ \cline{2-4} 0 & 0 & 1 & 2 \\ \cline{3-4} 0 & 0 & 0 & \frac{19}{2} \end{array}\right)$$

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if and only if $\alpha > 0$ and the matrix $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite.

Corollary: Positive definite matrices can be recognized by Gaussian elimination, but columns should be eliminated in the top to bottom manner by subtracting appropriate multiples of the pivot rows from the rows below, i.e. the order of the rows must not change nor the rows can be multiplied by a scalar.

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Example:

$$\begin{pmatrix} 4 & 2 & 0 & -1 \\ 2 & 2 & 2 & 2 \\ 0 & 2 & 5 & 7 \\ -1 & 2 & 7 & 20 \end{pmatrix} \sim\sim \begin{pmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 2 & 5 & 7 \\ 0 & \frac{5}{2} & 7 & \frac{79}{4} \end{pmatrix} \sim\sim \begin{pmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & \frac{27}{2} \end{pmatrix} \sim\sim \begin{pmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & \frac{19}{2} \end{pmatrix}$$

A recursive condition

Theorem: A block matrix $\boldsymbol{A} = \begin{array}{|c|c|} \hline \alpha & \boldsymbol{a}^H \\ \hline \boldsymbol{a} & \tilde{\boldsymbol{A}} \\ \hline \end{array}$ is positive definite

if and only if $\alpha > 0$ and the matrix $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite.

Proof: $\Leftarrow$ Let $\boldsymbol{x} \in \mathbb{C}^n \setminus \boldsymbol{0}$, denote $\boldsymbol{x}^T = \begin{array}{|c|c|} \hline x_1 & \tilde{\boldsymbol{x}}^T \\ \hline \end{array}, x_1 \in \mathbb{C}, \tilde{\boldsymbol{x}} \in \mathbb{C}^{n-1}$.

$$\boldsymbol{x}^H\boldsymbol{A}\boldsymbol{x} = \begin{array}{|c|c|} \hline \overline{x_1} & \tilde{\boldsymbol{x}}^H \\ \hline \end{array} \cdot \begin{array}{|c|c|} \hline \alpha & \boldsymbol{a}^H \\ \hline \boldsymbol{a} & \tilde{\boldsymbol{A}} \\ \hline \end{array} \cdot \begin{array}{|c|} \hline x_1 \\ \hline \tilde{\boldsymbol{x}} \\ \hline \end{array} = \alpha x_1\overline{x_1} + x_1\tilde{\boldsymbol{x}}^H\boldsymbol{a} + \overline{x_1}\boldsymbol{a}^H\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{x}}^H\tilde{\boldsymbol{A}}\tilde{\boldsymbol{x}}$$
$$-\frac{1}{\alpha}\tilde{\boldsymbol{x}}^H\boldsymbol{a}\boldsymbol{a}^H\tilde{\boldsymbol{x}} + \frac{1}{\alpha}\tilde{\boldsymbol{x}}^H\boldsymbol{a}\boldsymbol{a}^H\tilde{\boldsymbol{x}}$$
$$= \tilde{\boldsymbol{x}}^H(\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H)\tilde{\boldsymbol{x}} + (\sqrt{\alpha}\overline{x_1} + \frac{1}{\sqrt{\alpha}}\tilde{\boldsymbol{x}}^H\boldsymbol{a})(\sqrt{\alpha}x_1 + \frac{1}{\sqrt{\alpha}}\boldsymbol{a}^H\tilde{\boldsymbol{x}})$$

Both summands are nonnegative: $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite; and the next is the standard inner product of a vector with itself. At least one is strictly positive as otherwise $\boldsymbol{x} = \boldsymbol{0}$. Thus $\boldsymbol{x}^H\boldsymbol{A}\boldsymbol{x} > 0$.

$\Rightarrow$ For $\tilde{\boldsymbol{x}} \in \mathbb{C}^{n-1} \setminus \boldsymbol{0}$ we choose $x_1 = -\frac{1}{\alpha}\boldsymbol{a}^H\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}^T = \begin{array}{|c|c|} \hline x_1 & \tilde{\boldsymbol{x}}^T \\ \hline \end{array}$.

By our choice: $\sqrt{\alpha}x_1 + \frac{1}{\sqrt{\alpha}}\boldsymbol{a}^H\tilde{\boldsymbol{x}} = 0$.

Now $0 < \boldsymbol{x}^H\boldsymbol{A}\boldsymbol{x} = \tilde{\boldsymbol{x}}^H(\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H)\tilde{\boldsymbol{x}} + 0 \cdot 0$

Hence $\tilde{\boldsymbol{A}} - \frac{1}{\alpha}\boldsymbol{a}\boldsymbol{a}^H$ is positive definite.

Also $\boldsymbol{e}^{1H}\boldsymbol{A}\boldsymbol{e}^1 = \alpha > 0$.

Sylvester condition

Theorem: A Hermitian matrix $\boldsymbol{A}$ of order n is positive definite if and only if the matrices $\boldsymbol{A}_1, \ldots, \boldsymbol{A}_n$ have positive determinants, where $\boldsymbol{A}_i$ uses the first i rows and columns of $\boldsymbol{A}$.

Example:

$$|\boldsymbol{A}| = |\boldsymbol{A}_4| = \begin{vmatrix} 4 & 2 & 0 & -1 \\ 2 & 2 & 2 & 2 \\ 0 & 2 & 5 & 7 \\ -1 & 2 & 7 & 20 \end{vmatrix} = 38 > 0$$

$$|\boldsymbol{A}_3| = \begin{vmatrix} 4 & 2 & 0 \\ 2 & 2 & 2 \\ 0 & 2 & 5 \end{vmatrix} = 4 > 0$$

$$|\boldsymbol{A}_2| = \begin{vmatrix} 4 & 2 \\ 2 & 2 \end{vmatrix} = 4 > 0$$

$$|\boldsymbol{A}_1| = \det(4) = 4 > 0$$

All determinants are positive, thus the matrix $\boldsymbol{A}$ is positive definite.

Sylvester condition

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Proof: Use Gaussian elimination $\boldsymbol{A} \sim \cdots \sim \boldsymbol{A}'$ to test whether $\boldsymbol{A}$ is positive definite. Let $\alpha_1, \ldots, \alpha_n$ be the elements on the diagonal of the resulting upper triangular matrix $\boldsymbol{A}'$.
Since we have eliminated rows in the top-to-bottom manner, we have $\det(\boldsymbol{A}_i) = \det(\boldsymbol{A}'_i) = \prod_{j \le i} \alpha_j = \det(\boldsymbol{A}_{i-1})\alpha_i$.

$$\begin{aligned} \boldsymbol{A} \text{ is positive definite} &\Leftrightarrow \alpha_1, \ldots, \alpha_n > 0 \\ &\Leftrightarrow \det(\boldsymbol{A}_1), \ldots, \det(\boldsymbol{A}_n) > 0. \end{aligned}$$

Example:

$$\begin{array}{c} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \mathbf{A}_3 \\ \mathbf{A}_4 \end{array} \begin{vmatrix} 4 & 2 & 0 & -1 \\ 2 & 2 & 2 & 2 \\ 0 & 2 & 5 & 7 \\ -1 & 2 & 7 & 20 \end{vmatrix} = \begin{vmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 2 & 5 & 7 \\ 0 & \frac{5}{2} & 7 & \frac{79}{4} \end{vmatrix} = \begin{vmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & \frac{27}{2} \end{vmatrix} = \begin{vmatrix} 4 & 2 & 0 & -1 \\ 0 & 1 & 2 & \frac{5}{2} \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & \frac{19}{2} \end{vmatrix} \begin{array}{c} \mathbf{A}'_1 \\ \mathbf{A}'_2 \\ \mathbf{A}'_3 \\ \mathbf{A}'_4 \end{array}$$