Numerical Analysis
Matrix decompositions

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LU decomposition by Gaussian elimination

Let $A = [a_{kj}] \in \mathbf{M}_{N\times N}$ be a regular matrix, for which the Gaussian elimination can be performed *without swapping rows*.

LU decomposition

The matrix A can be uniquely decomposed in the following form:

$$A = LU$$

where L is a **normed lower triangular matrix** (i.e. $L_{kk} = 1$, and $L_{kj} = 0$, if $j > k$), and U is an **upper triangular matrix** (i.e. $U_{kj} = 0$, whenever $j < k$).

If a linear system $Ax = b$ should be solved with a lot of different right-hand sides b, then it is much cheaper to solve the pairs of equations instead: $Ly = b$, $Ux = y$, since only forward and backward substitutions have to be performed.

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Some useful statements

- The product of (normed) lower triangular matrix is (normed) lower triangular
- The product of (normed) upper triangular matrix is (normed) upper triangular
- The inverse of a (normed) lower triangular matrix is (normed) lower triangular (if exists)
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LU decomposition by Gaussian elimination

Performing the decomposition by Gaussian elimination: At the elimination by the kth row, subtract the kth row multiplied by $l_{m,k} := a_{m,k}/a_{k,k}$ from the mth row $(m = k+1, ..., N)$.

From these numbers $l_{m,k}$, the matrix L can be assembled:

$$L = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ l_{2,1} & 1 & 0 & \dots & 0 \\ l_{3,1} & l_{3,2} & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ l_{N,1} & l_{N,2} & l_{N,3} & \dots & 1 \end{pmatrix}$$

After the elimination steps, from the original matrix A, we arrive at the matrix U.

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After the elimination steps, from the original matrix A, we arrive at the matrix U.

LU decomposition, example

Determine the LU decomposition of the matrix

$$A = \begin{pmatrix} 2 & -6 & 10 \\ 2 & -5 & 3 \\ 3 & -2 & 1 \end{pmatrix}$$

LU decomposition, example

$$\begin{pmatrix} 2 & -6 & 10 \\ 2 & -5 & 3 \\ 3 & -2 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 \\ . & 1 & 0 \\ . & . & 1 \end{pmatrix}$$

$$\begin{pmatrix} 2 & -6 & 10 \\ 0 & 1 & -7 \\ 3 & -2 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ . & . & 1 \end{pmatrix}$$

$$\begin{pmatrix} 2 & -6 & 10 \\ 0 & 1 & -7 \\ 0 & 7 & -14 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ \frac{3}{2} & . & 1 \end{pmatrix}$$

$$\boxed{\begin{pmatrix} 2 & -6 & 10 \\ 0 & 1 & -7 \\ 0 & 0 & 35 \end{pmatrix} = U} \qquad \boxed{\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ \frac{3}{2} & 7 & 1 \end{pmatrix} = L}$$

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LU decomposition by matrix multiplication

In the previous example, first, write down the entries of L and U which are a priori known:

$$U = \begin{pmatrix} 2 & -6 & 10 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ \frac{3}{2} & \ell_{32} & 1 \end{pmatrix} \qquad \begin{pmatrix} 2 & -6 & 10 \\ 2 & -5 & 3 \\ 3 & -2 & 1 \end{pmatrix} = A$$

LU decomposition by matrix multiplication

Multiplying the 2nd row of L by the 2nd column of U, u_{22} can be computed: $u_{22} = 1$.

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LU decomposition by matrix multiplication

Multiplying the 3rd row of L by the 2nd column of U, ℓ_{32} can be computed: $\ell_{32} = 7$.

$$U = \begin{pmatrix} 2 & -6 & 10 \\ 0 & 1 & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

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Finally, multiplying the 3rd row of L by the 3rd column of U, u_{33} can be computed: $u_{33} = 35$.

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LU decomposition, numerical features

Computational cost

The necessary number of arithmetic operations of the LU decomposition of an $N \times N$ matrix is $\mathcal{O}(N^3)$.

Calculation of the determinant

Once the LU decomposition $A = LU$ has been performed, the determinant of A can be calculated as:

$$\det(A) = \det(L) \cdot \det(U) = u_{11} \cdot u_{22} \cdot \ldots \cdot u_{NN}$$

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The LDL^* factorization

Let $A \in \mathbf{M}_{N\times N}$ be a **self-adjoint, positive definite** matrix (which assures that the Gaussian elimination can be performed without swapping rows). Consider the LU decomposition of A:

$$A = LU$$

Denote by D the diagonal part of U, then $U = DU'$, where U' is a normed upper trianglular matrix. Since A is self-adjoint, the uniqueness of the LU decomposition implies that

$$U' = L^*$$

therefore

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LDL^* decomposition

Every self-adjoint, positive definite matrix A can be uniquely decomposed in the following form:

$$A = LDL^*$$

where L is a normed lower triangular matrix and D is a diagonal matrix, the diagonal entries of which are positive.

The Cholesky factorization

Let $A \in \mathbf{M}_{N\times N}$ be a self-adjoint, positive definite matrix with the LDL^* decomposition:

$$A = L_0 D L_0^*$$

Then

$$A = L_0\sqrt{D}\sqrt{D}L_0^* = (L_0\sqrt{D})\cdot(L_0\sqrt{D})^* =: LL^*$$

Cholesky decomposition

Every self-adjoint, positive definite matrix A can be uniquely decomposed in the following form:

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where L is a not necessarily normed lower triangular matrix, with positive diagonal elements.

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The number of necessary arithmetic operations of the Cholesky decomposition of an $N \times N$ self-adjoint, positive definite matrix is $\mathcal{O}(N^3)$.

The Cholesky decomposition is less sensitive to the roundoff errors than the LU decomposition.

If a linear system $Ax = b$ should be solved with a lot of different right-hand sides b, then it is cheaper to solve the pairs of equations instead: $Ly = b$, $L^*x = y$, since only forward and backward substitutions have to be performed.

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The Cholesky decomposition, example

$$A := \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$$

The LU decomposition (please check):

$$A = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & \frac{2}{3} & 2 \end{pmatrix} \cdot \begin{pmatrix} 2 & 1 & 0 \\ 0 & \frac{3}{2} & 1 \\ 0 & 0 & \frac{4}{3} \end{pmatrix}$$

Thus, the Cholesky decomposition: $A = L \cdot L^*$, where

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & \frac{2}{3} & 2 \end{pmatrix} \cdot \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{4}{3}} \end{pmatrix} = \begin{pmatrix} \sqrt{2} & 0 & 0 \\ \frac{\sqrt{2}}{2} & \sqrt{\frac{3}{2}} & 0 \\ 0 & \sqrt{\frac{2}{3}} & \frac{2}{\sqrt{3}} \end{pmatrix}$$

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Cholesky decomposition by matrix multiplication

In the previous example, first, write down the entries of L which are a priori known:

$$L^* = \begin{pmatrix} \ell_{11} & \ell_{21} & \ell_{31} \\ 0 & \ell_{22} & \ell_{32} \\ 0 & 0 & \ell_{33} \end{pmatrix}$$

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Cholesky decomposition by matrix multiplication

Multiplying the first row of L by the first column of L^*, ℓ_{11} can be computed: $\ell_{11} = \sqrt{2}$.

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Cholesky decomposition by matrix multiplication

Multiplying the 2nd and 3rd rows of L by the first column of L^*, ℓ_{21}, ℓ_{31} can be computed: $\ell_{21} = \sqrt{\frac{1}{2}}$, $\ell_{31} = 0$.

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Cholesky decomposition by matrix multiplication

Multiplying the 3rd row of L by the 2nd column of L^*, ℓ_{32} can be computed: $\ell_{32} = \sqrt{\frac{2}{3}}$.

$$L^* = \begin{pmatrix} \sqrt{2} & \sqrt{\frac{1}{2}} & 0 \\ 0 & \sqrt{\frac{3}{2}} & \ell_{32} \\ 0 & 0 & \ell_{33} \end{pmatrix}$$

$$L = \begin{pmatrix} \sqrt{2} & 0 & 0 \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} & 0 \\ 0 & \ell_{32} & \ell_{33} \end{pmatrix} \quad \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix} = A$$

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Finally, multiplying the 3rd row of L by the 3rd column of L^*, ℓ_{33} can be computed: $\ell_{33} = \sqrt{\frac{4}{3}}$.

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The Gram-Schmidt orthogonalization

Let $a_1, a_2, ..., a_N \in \mathbf{R}^N$ be linearly independent vectors. Define $\tilde{e}_1 := a_1$, $e_1 := \frac{\tilde{e}_1}{||\tilde{e}_1||}$, and for $k = 2, 3, ..., N$:

$$\tilde{e}_k := a_k - \sum_{j=1}^{k-1} \langle a_k, e_j \rangle e_j, \qquad e_k := \frac{\tilde{e}_k}{||\tilde{e}_k||}$$

Gram-Schmidt orthogonalization

The vectors $e_1, e_2, ..., e_N$ form an **orthonormal vector system** (i.e. $\langle e_k, e_j \rangle = 0$, if $k \neq j$, and $||e_k|| = 1$), and the vector systems $a_1, a_2, ..., a_k$ and $e_1, e_2, ..., e_k$ generate the same subspace of $\mathbf{R}^N$ for all $k = 1, 2, ..., N$.

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Orthogonal matrices

The matrix $A \in \mathbf{M}_{N\times N}$ is called **orthogonal**, if its column vectors form an orthonormal system in $\mathbf{R}^N$.

Example: The 2-by-2 matrix $A := \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix}$ is an orthogonal matrix.

The inverse of orthogonal matrices can be computed in an extremely simple way:

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Every regular matrix $A \in \mathbf{M}_{N\times N}$ can be uniquely decomposed in the form $A = QR$, where Q is an orthogonal matrix, R is an upper triangular matrix with positive diagonal entries.

Denote by $a_1, a_2, ..., a_N$ its column vectors. Consider the orthonormal basis $e_1, e_2, ..., e_N$ obtained from $a_1, a_2, ..., a_N$ by a Gram-Schmidt orthogonalization. Then

$$Q = \left(\begin{array}{c|c|c|c} e_1 & e_2 & \dots & e_N \end{array} \right), \qquad R = \begin{pmatrix} r_{11} & r_{12} & r_{13} & \dots \\ 0 & r_{22} & r_{23} & \dots \\ 0 & 0 & r_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

where $r_{kj} := \langle e_k, a_j \rangle$

After performing the QR decomposition, the solution of the linear system $Ax = b$ is extremely simple with low computational cost:

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The QR decomposition, example

Compute the QR decomposition of the matrix $A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 3 \end{pmatrix}$.

First, $a_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \quad a_3 = \begin{pmatrix} 1 \\ 0 \\ 3 \end{pmatrix}$.

Next, perform a Gram-Schmidt-ortogonalization for these vectors:

$$\tilde{e}_1 = a_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad e_1 = \boxed{\begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix}}$$

$$\tilde{e}_2 = a_2 - \langle a_2, e_1 \rangle \cdot e_1 = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \quad e_2 = \boxed{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}$$

$$\tilde{e}_3 = a_3 - \langle a_3, e_1 \rangle \cdot e_1 - \langle a_3, e_2 \rangle \cdot e_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \quad e_3 = \boxed{\begin{pmatrix} -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix}}$$

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Thus we have obtained: $\boxed{Q = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \end{pmatrix}}$

Moreover:

$r_{11} = ||\tilde{e}_1|| = \sqrt{2}, \qquad r_{12} = \langle e_1, a_2 \rangle = 0, \qquad r_{13} = \langle e_1, a_3 \rangle = 2\sqrt{2}$

$r_{22} = ||\tilde{e}_2|| = 2, \qquad r_{23} = \langle e_2, a_3 \rangle = 0$

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and therefore: $\boxed{R = \begin{pmatrix} \sqrt{2} & 0 & 2\sqrt{2} \\ 0 & 2 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}}$

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