

Math 6610: Analysis of Numerical Methods, I

The LU and Cholesky decompositions

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Resources: Trefethen and Bau 1997, Lectures 20, 21, 23
Atkinson 1989, Chapter 1
Salgado and Wise 2022, Chapter 3

Let $A \in \mathbb{C}^{n \times n}$ be an invertible matrix, and let $b \in \mathbb{C}^n$ be any vector.

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One "standard" way to do this starts by forming the *augmented* rectangular matrix

$$(A \ b) \in \mathbb{C}^{n \times (n+1)},$$

and proceeds to perform elimination steps to transform the left $n \times n$ block into the identity matrix.

If we record the row operations needed to perform Gaussian elimination, then we can work *only* on the matrix \mathbf{A} .

Consider a matrix \mathbf{A} with columns $(\mathbf{a}_j)_{j=1}^n$:

$$\mathbf{A} = \left(\begin{array}{c|c|ccc|c} & & & & & \\ & & & & & \\ \mathbf{a}_1 & & \mathbf{a}_2 & & \cdots & & \mathbf{a}_n & & \\ & & & & & & & & \end{array} \right), \quad \mathbf{a}_j = \begin{pmatrix} a_{j,1} \\ a_{j,2} \\ \vdots \\ a_{j,n} \end{pmatrix}$$

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If $a_{1,1} \neq 0$, then by standard Gaussian elimination, we replace row j with itself minus a scaled version of row 1 to eliminate entries in column 1.

I.e., if \mathbf{r}_j^* is row j of \mathbf{A} , then for $j > 1$, replace row j with,

$$\tilde{\mathbf{r}}_j^* = \mathbf{r}_j^* - \frac{a_{j,1}}{a_{1,1}} \mathbf{r}_1^*$$

In particular, this shows that \mathbf{r}_j can be reconstructed in terms of $\tilde{\mathbf{r}}_j$ and \mathbf{r}_1 .

After row operations that transform the first column to a multiple of e_1 , we have

$$\mathbf{A} = \mathbf{L}_1 \mathbf{A}_2, \quad \mathbf{L}_1 = \left(\begin{array}{c|cc} | & - & \mathbf{0}_{1 \times (n-1)} & - \\ \ell & & \mathbf{I}_{(n-1) \times (n-1)} & \\ | & & & \end{array} \right),$$

with \mathbf{A}_2 the matrix

$$\mathbf{A}_2 = \left(\begin{array}{c|ccc} a_{1,1} & | & & | \\ 0 & \mathbf{a}_2^{(2)} & \cdots & \mathbf{a}_n^{(2)} \\ \vdots & & & \\ 0 & | & & | \end{array} \right).$$

If we continue triangular elimination from A_2 , until the last column we obtain,

$$A = L_1 \cdots L_{n-1} A_n,$$

where A_n is an upper-triangular matrix, and each L_j has the form,

$$L_j = \left(\begin{array}{c|ccc|ccc} & & & & & & & \\ e_1 & \cdots & e_{j-1} & \ell_j & e_{j+1} & \cdots & e_n \\ & & & & & & & \end{array} \right),$$

where ℓ_j is a vector with j th component $\ell_{j,j} = 1$, and $\ell_{j,k} = 0$ for $k < j$.

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$$L_j = \begin{pmatrix} \begin{array}{c} | \\ e_1 \\ | \end{array} & \cdots & \begin{array}{c} | \\ e_{j-1} \\ | \end{array} & \begin{array}{c} | \\ \ell_j \\ | \end{array} & \begin{array}{c} | \\ e_{j+1} \\ | \end{array} & \cdots & \begin{array}{c} | \\ e_n \\ | \end{array} \end{pmatrix},$$

where ℓ_j is a vector with j th component $\ell_{j,j} = 1$, and $\ell_{j,k} = 0$ for $k < j$. Note that each L_j is lower triangular, and one can show that

$$L_j L_{j+1} = \begin{pmatrix} e_1 & \cdots & e_{j-1} & \ell_j & \ell_{j+1} & e_{j+2} & \cdots & e_n \end{pmatrix},$$

so that $L := \prod_{j=1}^{n-1} L_j$ is also upper-triangular.

We have just shown that, if all our elimination steps successfully complete, then

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How can the steps fail?

Theorem

\mathbf{A} has an LU decomposition if and only if $\det \mathbf{A}_j \neq 0$ for all $j = 1, \dots, n$, where \mathbf{A}_j is the principal (upper-left) $j \times j$ submatrix of \mathbf{A} .

The LU factorization/decomposition has several uses;

- It's how we solve linear systems
- If an LU factorization for A is available, then solving $Ax = b$ requires only $\mathcal{O}(n^2)$ operations.
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“Standard” Gaussian elimination fails in some cases, e.g., with

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

The standard approach to “fixing” this problem is pivoting, which interchanges rows and/or columns.

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This results in the decomposition,

$$A = P_1 L_1 P_2 L_2 \cdots P_{n-1} L_{n-1} U,$$

where P_j is a permutation matrix that permutes row j with row k for some $k \geq j$.

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where P_j is a permutation matrix that permutes row j with row k for some $k \geq j$. One can show that $L_j P_k = P_k \tilde{L}_j$ if $j < k$ for some other lower-triangular matrix \tilde{L}_j , so that

$$A = \left(\prod_{j=1}^{n-1} P_j \right) \left(\prod_{j=1}^{n-1} \tilde{L}_j \right) U.$$

In fact, we can show that this *row pivoting* strategy always works.

Theorem

If $A \in \mathbb{C}^{n \times n}$ is invertible, then there exists

- a permutation matrix P ,*
- a lower-triangular matrix L ,*
- an upper-triangular matrix U ,*

such that

$$PA = LU$$

Row pivoting is not the only option.

For example, *full* pivoting permutes *both* lower rows and rightmost columns in search of a maximum-magnitude pivot.

$$A = P_1 L_1 P_2 L_2 \cdots P_{n-1} L_{n-1} U Q_{n-1} Q_{n-2} \cdots Q_1,$$

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An alternative is *rook pivoting*, which performs a permutation similar to the above, except that at elimination step j , the maximum is sought *only* over row j and column j . All flavors of LU factorizations require $\mathcal{O}(n^3)$ complexity with explicit, small multiplying constant.

But the choice of pivoting can substantially affect the actual runtime (the constant).

Assume $A \in \mathbb{C}^{n \times n}$ is Hermitian positive definite.

Our investigation of LU decompositions specializes considerably in this case.

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First we note some properties of A :

- A is invertible
- The diagonal entries of A are real and strictly positive
- If $B \in \mathbb{C}^{m \times n}$ with $m \leq n$ is of full rank, then BAB^* is positive-definite

A general positive-definite matrix \mathbf{A} has the form

$$\mathbf{A} = \begin{pmatrix} a & - & \mathbf{v}^* & - \\ | & & & \\ \mathbf{v} & & \mathbf{A}_2 & \\ | & & & \end{pmatrix}.$$

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Consider performing elimination on A :

$$A = L_1 B^* = \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ \frac{\mathbf{v}}{a} & & I & \\ | & & & \end{pmatrix} \begin{pmatrix} a & - & \mathbf{v}^* & - \\ | & & & \\ 0 & & A_2 - \frac{\mathbf{v}\mathbf{v}^*}{a} & \\ | & & & \end{pmatrix}$$

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i.e.,

$$A = L_1 \left(\begin{array}{c|cc} a & - & 0 & - \\ \hline 0 & & A_2 - \frac{vv^*}{a} & \end{array} \right) L_1^* = \tilde{L}_1 \left(\begin{array}{c|cc} 1 & - & 0 & - \\ \hline 0 & & A_2 - \frac{vv^*}{a} & \end{array} \right) \tilde{L}_1^*.$$

$$A = \tilde{L}_1 \begin{pmatrix} 1 & - & 0 & - \\ | & & & \\ 0 & A_2 - \frac{vv^*}{a} & & \\ | & & & \end{pmatrix} \tilde{L}_1^*.$$

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Thus, we can repeat this process:

$$\begin{aligned} A &= \left(\tilde{L}_1 \tilde{L}_2 \cdots \tilde{L}_{n-1} \right) \left(\tilde{L}_1 \tilde{L}_2 \cdots \tilde{L}_{n-1} \right)^* \\ &=: LL^*. \end{aligned}$$

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Theorem

Every Hermitian positive definite matrix A has a unique symmetric LU, or Cholesky, decomposition: $A = LL^$, where L is lower-triangular and invertible.*

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However, pivoted Cholesky decompositions have another use:

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*Every Hermitian positive semi-definite matrix A has a pivoted Cholesky decomposition: $A = PLL^*P^*$, where L is lower-triangular but need not be invertible. This decomposition is in general not unique.*

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Why do we care about Cholesky decompositions? For positive-definite matrices:

- Not having to deal with pivoting is of considerable computational savings (but doesn't change asymptotic complexity)
- The Cholesky decomposition provides a “whitening” transform, e.g., for $x \mapsto x^*Ax$.
- Low-rank updates of Cholesky factors are (very) useful.

A minor generalization of LU for a generic matrix: If A is invertible, then we can always write,

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where P is a permutation matrix.

By construction:

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Let D be a diagonal matrix with the pivot entries of U , then we can write,

$$PA = LD\tilde{U},$$

where both L and U have ones on the diagonal. This is the (pivoted) LDU decomposition of A .
(There are some niche cases when doing this decomposition of A is slightly preferable.)

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For Hermitian positive semi-definite matrices, we can write

$$PAP^* = LDL^*$$

(Or without permutations if A is positive definite.) This is the LDL^T decomposition of A .

-  Atkinson, Kendall (1989). *An Introduction to Numerical Analysis*. New York: Wiley. ISBN: 978-0-471-62489-9.
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-  Trefethen, Lloyd N. and David Bau (1997). *Numerical Linear Algebra*. SIAM: Society for Industrial and Applied Mathematics. ISBN: 0-89871-361-7.