

LU and Cholesky decompositions. J. Demmel,
Chapter 2.7

Gaussian Elimination

The Algorithm — Overview

Solving $Ax = b$ using Gaussian elimination.

- 1 Factorize A into $A = PLU$

Permutation Unit lower triangular Non-singular upper triangular

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② Solve $PLUx = b$ (for LUx) :

$$LUx = P^{-1}b$$

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- 3 Solve $LUx = P^{-1}b$ (for Ux) by forward substitution:

$$Ux = L^{-1}(P^{-1}b).$$

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- 3 Solve $LUx = P^{-1}b$ (for Ux) by forward substitution:

$$Ux = L^{-1}(P^{-1}b).$$

- 4 Solve $Ux = L^{-1}(P^{-1}b)$ by backward substitution:

$$x = U^{-1}(L^{-1}P^{-1}b).$$

Example of LU factorization

We factorize the following 2-by-2 matrix:

$$\begin{bmatrix} 4 & 3 \\ 6 & 3 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix}. \quad (1)$$

One way to find the LU decomposition of this simple matrix would be to simply solve the linear equations by inspection. Expanding the matrix multiplication gives

$$\begin{aligned} l_{11} \cdot u_{11} + 0 \cdot 0 &= 4, \\ l_{11} \cdot u_{12} + 0 \cdot u_{22} &= 3, \\ l_{21} \cdot u_{11} + l_{22} \cdot 0 &= 6, \\ l_{21} \cdot u_{12} + l_{22} \cdot u_{22} &= 3. \end{aligned} \quad (2)$$

This system of equations is underdetermined. In this case any two non-zero elements of L and U matrices are parameters of the solution and can be set arbitrarily to any non-zero value. Therefore, to find the unique LU decomposition, it is necessary to put some restriction on L and U matrices. For example, we can conveniently require the lower triangular matrix L to be a unit triangular matrix (i.e. set all the entries of its main diagonal to ones).

Then the system of equations has the following solution:

$$\begin{aligned}l_{21} &= 1.5, \\u_{11} &= 4, \\u_{12} &= 3, \\u_{22} &= -1.5.\end{aligned}\tag{3}$$

Substituting these values into the LU decomposition above yields

$$\begin{bmatrix} 4 & 3 \\ 6 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1.5 & 1 \end{bmatrix} \begin{bmatrix} 4 & 3 \\ 0 & -1.5 \end{bmatrix}.\tag{4}$$

Gaussian Elimination

The Algorithm — uniqueness of factorization

Definition

The leading j -by- j principal submatrix of A is $A(1 : j, 1 : j)$.

Theorem 2.4.

The following two statements are equivalent:

- 1. There exists a unique unit lower triangular L and non-singular upper triangular U such that $A = LU$.*
- 2. All leading principal submatrices of A are non-singular.*

Gaussian Elimination

The Algorithm

Algorithm 2.2

LU factorization with pivoting:

for $i = 1$ to $n-1$

apply permutations so $a_{ii} \neq 0$ (permute L, U)

/ for example for GEPP, swap rows j and i of A and of L
where $|a_{ji}|$ is the largest entry in $|A(i : n, i)|$;*

*for GECP, swap rows j and i of A and of L , and columns k
and i of A and U , where $|a_{jk}|$ is the largest entry in*

*$|A(i : n, i : n)|$ */*

/ compute column i of L */*

for $j=i+1$ to n

$$l_{ji} = \frac{a_{ji}}{a_{ii}}$$

end for

/ compute row j of U */*

for $j=i$ to n

$$u_{ij} = a_{ij} \quad \text{end for}$$

Gaussian Elimination

The Algorithm

Algorithm 2.2

```
/* update  $A_{22}$  */  
for  $j=i+1$  to  $n$   
    for  $k=i+1$  to  $n$   
         $a_{jk} = a_{jk} - l_{ji} * u_{ik}$   
    end for  
end for  
end for
```

Gaussian Elimination

The Algorithm

Algorithm 2.3

LU factorization with pivoting, overwriting L and U on A:

for i=1 to n-1

apply permutations (see Algorithm 2.2.)

for j=i+1 to n

$$a_{ji} = \frac{a_{ji}}{a_{ii}}$$

end for

for j=i+1 to n

for k=i+1 to n

$$a_{jk} = a_{jk} - a_{ji} * a_{ik}$$

end for

end for

end for

Gaussian Elimination

The Algorithm

Algorithm 2.4

LU factorization with pivoting, overwriting L and U on A, using Matlab notations:

for i=1 to n-1

apply permutations(see algorithm 2.2.)

$A(i+1:n,i)=A(i+1:n,i)/A(i,i)$

$A(i+1:n,i,i+1:n)=$

*$A(i+1:n,i+1:n)-A(i+1:n,i)*A(i,i+1:n)$*

end for

2.7.1. Real Symmetric Positive Definite Matrices

Recall that a real matrix A is s.p.d. if and only if $A = A^T$ and $x^T A x > 0$ for all $x \neq 0$. In this section we will show how to solve $Ax = b$ in half the time and half the space of Gaussian elimination when A is s.p.d.

PROPOSITION 2.2.

1. *If X is nonsingular, then A is s.p.d. if and only if $X^T A X$ is s.p.d.*
2. *If A is s.p.d. and H is any principal submatrix of A ($H = A(j : k, j : k)$ for some $j \leq k$), then H is s.p.d.*
3. *A is s.p.d. if and only if $A = A^T$ and all its eigenvalues are positive.*
4. *If A is s.p.d., then all $a_{ii} > 0$, and $\max_{ij} |a_{ij}| = \max_i a_{ii} > 0$.*
5. *A is s.p.d. if and only if there is a unique lower triangular nonsingular matrix L , with positive diagonal entries, such that $A = LL^T$. $A = LL^T$ is called the Cholesky factorization of A , and L is called the Cholesky factor of A .*

ALGORITHM 2.11. *Cholesky algorithm:*

for $j = 1$ *to* n

$$l_{jj} = (a_{jj} - \sum_{k=1}^{j-1} l_{jk}^2)^{1/2}$$

for $i = j + 1$ *to* n

$$l_{ij} = (a_{ij} - \sum_{k=1}^{j-1} l_{ik}l_{jk})/l_{jj}$$

end for

end for

If A is not positive definite, then (in exact arithmetic) this algorithm will fail by attempting to compute the square root of a negative number or by dividing by zero; this is the cheapest way to test if a symmetric matrix is positive definite.