Vv417 Lecture 7

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- Since $\mathbf{A}$ is nonsingular, we could compute

$$\mathbf{A}^{-1}$$

however, Gaussian elimination with back substitution (GS) is faster

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

despite having covered Cramer's rule and the simple-looking formula

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

Q: What should we do if we are forced to find the inverse of a large matrix?

Q: How many arithmetic operations are needed to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$ using GS?

Q: How many arithmetic operations are needed to find $\mathbf{A}^{-1}$?

Q: How many arithmetic operations are needed to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$ by using $\mathbf{A}^{-1}$?

- In practice, there is hardly ever a good reason to invert a matrix,

$$\mathbf{A}^{-1}$$

and Cramer's rule is only practical for a very small or a very special system.

Q: Shall we compute the inverse of $\mathbf{A}$ when solving a sequence of systems,

$$\mathbf{A}\mathbf{x}_1 = \mathbf{b}_1, \quad \mathbf{A}\mathbf{x}_2 = \mathbf{b}_2, \quad \mathbf{A}\mathbf{x}_3 = \mathbf{b}_3, \quad \ldots, \quad \mathbf{A}\mathbf{x}_k = \mathbf{b}_k$$

each of which has the same coefficient matrix $\mathbf{A}$?

- An efficient way is to form the following augmented matrix

$$\left[\begin{array}{c|ccccc} \mathbf{A} & \mathbf{b}_1 & \mathbf{b}_2 & \mathbf{b}_3 & \cdots & \mathbf{b}_k \end{array}\right]$$

and apply Gaussian elimination with back substitution to it.

Q: Have you seen any similar approach before?

- This approach allows us to solve all k systems at once just like when finding

$$\mathbf{A}^{-1}$$

- Applying Gaussian elimination with back substitution to,

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{I} \end{array}\right] = \left[\begin{array}{c|cccc} \mathbf{A} & \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_n \end{array}\right]$$

is far more efficient than using the adjoint method

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})} \operatorname{adj}(\mathbf{A})$$

- In fact, even if you have computed $\mathbf{A}^{-1}$, we still prefer avoid using it to solve

$$\mathbf{Ax} = \mathbf{b}$$

since performing the matrix multiplication is numerically less accurate.

Q: Is there an efficient way to avoid computing and storing

$$\mathbf{A}^{-1}$$

if we want to solve a sequence of systems,

$$\mathbf{A}\mathbf{x}_1 = \mathbf{b}_1, \quad \mathbf{A}\mathbf{x}_2 = \mathbf{b}_2, \quad \mathbf{A}\mathbf{x}_3 = \mathbf{b}_3, \quad \dots, \quad \mathbf{A}\mathbf{x}_k = \mathbf{b}_k$$

where $\mathbf{b}_1$ is known in advance, but $\mathbf{b}_2$ is only known once

$$\mathbf{x}_1$$

becomes available and $\mathbf{b}_3$ in turn only becomes available once

$$\mathbf{x}_2$$

is available and etc., that is, we must solve the systems sequentially.

- Unless $\mathbf{A}$ is small, computing and storing $\mathbf{A}^{-1}$ is unwise even in this case.

- Suppose $\mathbf{U}$ is an upper triangular matrix. Recall it is not necessary to obtain

$$\mathrm{rref}\,(\mathbf{U})$$

in order to solve a linear system

$$\mathbf{U}\mathbf{x} = \mathbf{y}$$

- If all diagonal elements of $\mathbf{U}$ are nonzero, then the solution can be found

$$x_n = \frac{y_n}{u_{nn}}; \qquad x_i = \frac{\left(y_i - \displaystyle\sum_{j=i+1}^{n} u_{ij} x_j\right)}{u_{ii}} \qquad \text{for} \quad i = n-1, \ldots, 1.$$

by back substitution. A similar procedure, known as forward substitution, can be applied when we have a lower triangular matrix $\mathbf{L}$.

Q: How many arithmetic operations does the forward substitution use?

- Now consider a more general linear system

$$\mathbf{Ax} = \mathbf{b}$$

in which the coefficient matrix $\mathbf{A}$ is given by

$$\mathbf{A} = \mathbf{LU}$$

where $\mathbf{L}$ is lower triangular and $\mathbf{U}$ is upper triangular with nonzero diagonals.

- In this case, the system can be broken into two systems by introducing

$$\mathbf{y} = \mathbf{Ux} \implies \mathbf{LUx} = \mathbf{b} \implies \begin{matrix} \mathbf{Ly} = \mathbf{b} \\ \mathbf{Ux} = \mathbf{y} \end{matrix}$$

both of which can be solved using either forward/back substitution.

Additions/Subtractions	Multiplications/Divisions
$\dfrac{n^2 - n}{2}$	$\dfrac{n^2 + n}{2}$

Definition

Let $\mathbf{A}$ a square matrix. An LU decomposition of $\mathbf{A}$ is a decomposition of $\mathbf{A}$ as

$$\mathbf{A} = \mathbf{L}\mathbf{U}$$

where $\mathbf{L}$ is lower triangular and $\mathbf{U}$ is upper triangular.

- In terms of solving the following sequential problem

$$\mathbf{A}\mathbf{x}_1 = \mathbf{b}_1, \quad \mathbf{A}\mathbf{x}_2 = \mathbf{b}_2, \quad \mathbf{A}\mathbf{x}_3 = \mathbf{b}_3, \quad \ldots, \quad \mathbf{A}\mathbf{x}_k = \mathbf{b}_k$$

  the idea is to compute and store matrices $\mathbf{L}$ and $\mathbf{U}$, then solve a sequence of

$$\begin{aligned} \mathbf{L}\mathbf{y}_i &= \mathbf{b}_i \\ \mathbf{U}\mathbf{x}_i &= \mathbf{y}_i \end{aligned} \qquad \text{for} \quad i = 1, 2, \ldots, k$$

  using either Forward/back Substitution.

Q: In additional to efficiency, can you think of another reason for using LU?

Matlab

Command Window

```
>>
>> N = 5;
>> x = [2 1 zeros(1, N-2)]

x =

     2     1     0     0     0

>> A = toeplitz(x,x)
% a Toeplitz matrix is
% a diagonal constant matrix

A =

     2     1     0     0     0
     1     2     1     0     0
     0     1     2     1     0
     0     0     1     2     1
     0     0     0     1     2

>>
```

Command Window

```
>>
>> inv(A)

ans =

    0.8333   -0.6667    0.5000   -0.3333    0.1667
   -0.6667    1.3333   -1.0000    0.6667   -0.3333
    0.5000   -1.0000    1.5000   -1.0000    0.5000
   -0.3333    0.6667   -1.0000    1.3333   -0.6667
    0.1667   -0.3333    0.5000   -0.6667    0.8333

>> [L,U] = lu(A)

L =

    1.0000         0         0         0         0
    0.5000    1.0000         0         0         0
         0    0.6667    1.0000         0         0
         0         0    0.7500    1.0000         0
         0         0         0    0.8000    1.0000


U =

    2.0000    1.0000         0         0         0
         0    1.5000    1.0000         0         0
         0         0    1.3333    1.0000         0
         0         0         0    1.2500    1.0000
         0         0         0         0    1.2000

>>
```

- Because both forward and back substitution require only

Additions/Subtractions	Multiplications/Divisions
$\frac{n^2 - n}{2}$	$\frac{n^2 + n}{2}$

whereas Gaussian elimination with back substitution in this context requires

Additions/Subtractions	Multiplications/Divisions
$\frac{2n^3 + 3n^2 - 5n}{6}$	$\frac{2n^3 + 6n^2 - 2n}{6}$

changes in the right-hand side,

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

can be handled quite efficiently by computing and storing $\mathbf{L}$ and $\mathbf{U}$.

- It turns out that $\mathbf{L}$ and $\mathbf{U}$ can be stored in a single $n \times n$ matrix. If $\mathbf{A}$ is sparse, it may be further reduced, in contrast to the difficulty of storing $\mathbf{A}^{-1}$.

Q: Given an $n \times n$ matrix, how to compute $\mathbf{A} = \mathbf{LU}$?

Q: Does an LU decomposition always exist for an arbitrary $n \times n$ matrix?

Q: Are $\mathbf{L}$ and $\mathbf{U}$ unique for a given matrix $\mathbf{A}$?

- Recall the sequence of row operations from Gaussian elimination produce

$$\mathbf{E}_k \cdots \mathbf{E}_2 \mathbf{E}_1 \mathbf{A} = \mathbf{U}$$

$$\mathbf{A} = \mathbf{E}_1^{-1} \mathbf{E}_2^{-1} \cdots \mathbf{E}_k^{-1} \mathbf{U}$$

- Consider the sequence of elementary matrices from Gaussian elimination for

$$\mathbf{E}_{(1)1,3}\mathbf{E}_{(-2)1,2} \underbrace{\begin{bmatrix} 2 & 1 & 3 \\ 4 & -1 & 3 \\ -2 & 5 & 5 \end{bmatrix}}_{\mathbf{A}} \sim \mathbf{E}_{(2)2,3} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -3 & -3 \\ 0 & 6 & 8 \end{bmatrix} = \underbrace{\begin{bmatrix} 2 & 1 & 3 \\ 0 & -3 & -3 \\ 0 & 0 & 2 \end{bmatrix}}_{\mathbf{U}}$$

$$\implies \mathbf{A} = \mathbf{E}_{(-2)1,2}^{-1}\mathbf{E}_{(1)1,3}^{-1}\mathbf{E}_{(2)2,3}^{-1}\mathbf{U}$$

$$= \mathbf{E}_{(2)1,2}\mathbf{E}_{(-1)1,3}\mathbf{E}_{(-2)2,3}\mathbf{U}$$

- Computing the product, we have

$$\begin{aligned}\mathbf{A} &= \mathbf{E}_{(2)1,2}\mathbf{E}_{(-1)1,3}\mathbf{E}_{(-2)2,3}\mathbf{U} \\ &= \begin{bmatrix}1 & 0 & 0\\ 2 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ -1 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & -2 & 1\end{bmatrix}\mathbf{U} \\ &= \begin{bmatrix}1 & 0 & 0\\ 2 & 1 & 0\\ -1 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & -2 & 1\end{bmatrix}\mathbf{U} = \underbrace{\begin{bmatrix}1 & 0 & 0\\ 2 & 1 & 0\\ -1 & -2 & 1\end{bmatrix}}_{\mathbf{L}}\mathbf{U}\end{aligned}$$

- Again one does not actually perform those matrix multiplications in practice,
  - The diagonals of $\mathbf{L}$ is always 1.
  - Elements below the diagonal of $\mathbf{L}$ is the multiplier

$$\ell_{ij} = \frac{a_{ij}^{(j)}}{a_{jj}^{(j)}}$$

used to create the ijth zero during Gaussian elimination.

Matlab

```matlab
function [L, U] = ludecomp(A)
%% Applying naive Doolittle algorithm to find LU decomposition
%
% A is an n by n matrix, for which LU exists
% L is a lower triangular matrix
% U is an upper triangular matrix such that A = LU

n = size(A,1); % Find number of rows
L = eye(n); % Taking care of diagonal and upper half

for j = 1:n
    L(j+1:n, j) = A(j+1:n, j) / A(j,j); % Multiplier

    for i = j+1:n
        A(i,:) = A(i,:) - L(i,j) * A(j,:); % Create zeros underneath
    end
end

U = A;

end
```

Command Window

```
>>
>> A = [ 2 1 3; 4 -1 3; -2 5 5]

A =

     2     1     3
     4    -1     3
    -2     5     5

>> [L, U] = ludecomp(A)

L =

     1     0     0
     2     1     0
    -1    -2     1


U =

     2     1     3
     0    -3    -3
     0     0     2

>> L*U

ans =

     2     1     3
     4    -1     3
    -2     5     5

>>
```

Q: Does Doolittle algorithm always work?

- Consider the following matrix again

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 3 \\ 4 & 2 & 1 \\ 6 & -3 & 4 \end{bmatrix}$$

for which we have the following when computing $\det(\mathbf{A})$

$$\begin{aligned}
\mathbf{A} &= \mathbf{E}_{(2)1,2}\mathbf{E}_{(3)1,3}\mathbf{E}_{3,2}\mathbf{U} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -6 & -5 \\ 0 & 0 & -5 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -6 & -5 \\ 0 & 0 & -5 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -6 & -5 \\ 0 & 0 & -5 \end{bmatrix}
\end{aligned}$$

Q: What do the above two examples seem to suggest?

Theorem

If $\mathbf{A}$ is an $n \times n$ matrix such that only Type III operations are used when applying Gaussian elimination to reduce $\mathbf{A}$ to an upper triangular matrix $\mathbf{U}$, then

$$\mathbf{A} = \mathbf{LU}$$

where $\mathbf{L}$ is a lower triangular matrix with unit diagonal elements.

Q: Given square matrix $\mathbf{A}$ has an LU decomposition, are $\mathbf{L}$ and $\mathbf{U}$ unique?

- Let $\mathbf{D}$ be a invertible diagonal matrix that is not the identity matrix, and

$$\begin{aligned} \mathbf{A} &= \mathbf{LU} && && \\ \mathbf{A} &= \mathbf{LD}\tilde{\mathbf{U}} && \text{where} && \tilde{\mathbf{U}} = \mathbf{D}^{-1}\mathbf{U} \\ \mathbf{A} &= \tilde{\mathbf{L}}\tilde{\mathbf{U}} && \text{where} && \tilde{\mathbf{L}} = \mathbf{LD} \end{aligned}$$

- It is clear that $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{U}}$ are upper and lower triangular, respectively, and

$$\mathbf{L} \neq \tilde{\mathbf{L}} \qquad \text{and} \qquad \mathbf{L} \neq \tilde{\mathbf{L}}$$

Theorem

If $\mathbf{A}$ is an invertible matrix and following decomposition exists,

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{D}\hat{\mathbf{U}}$$

where $\hat{\mathbf{L}}$ and $\hat{\mathbf{U}}$ are upper and lower triangular with unit diagonals, and

$$\mathbf{D}$$

is a diagonal matrix, then the above decomposition is unique.

Proof

- Firstly, since $\mathbf{A}$ is invertible, $\hat{\mathbf{L}}$, $\mathbf{D}$ and $\hat{\mathbf{U}}$ must be invertible,

$$\mathbf{A}^{-1} = \hat{\mathbf{U}}^{-1}\mathbf{D}^{-1}\hat{\mathbf{L}}^{-1}$$

  thus $\mathbf{D} = \mathrm{diag}\left(d_1, d_2, \ldots, d_n\right)$ cannot have zero diagonal elements

$$\mathbf{D}^{-1} = \mathrm{diag}\left(\frac{1}{d_1}, \frac{1}{d_2}, \cdots, \frac{1}{d_n}\right)$$

Proof

- Suppose there are two distinct decompositions of form $\mathbf{A} = \hat{\mathbf{L}}\mathbf{D}\hat{\mathbf{U}}$ for $\mathbf{A}$

$$\mathbf{A} = \mathbf{L}_1\mathbf{D}_1\mathbf{U}_1 \qquad \text{and} \qquad \mathbf{A} = \mathbf{L}_2\mathbf{D}_2\mathbf{U}_2$$

- Consider the following product,

$$\mathbf{L}_1^{-1}\mathbf{A}\mathbf{U}_2^{-1} \implies \mathbf{L}_1^{-1}(\mathbf{L}_1\mathbf{D}_1\mathbf{U}_1)\mathbf{U}_2^{-1} = \mathbf{L}_1^{-1}(\mathbf{L}_2\mathbf{D}_2\mathbf{U}_2)\mathbf{U}_2^{-1}$$

$$\mathbf{D}_1\mathbf{U}_1\mathbf{U}_2^{-1} = \mathbf{L}_1^{-1}\mathbf{L}_2\mathbf{D}_2$$

- The inverse of upper/lower triangular matrices is upper/lower triangular, and the product of upper/lower triangular matrices is upper/lower triangular, so

$$\begin{array}{ll} \mathbf{D}_1\mathbf{U}_1\mathbf{U}_2^{-1} & \text{is upper triangular} \\ \mathbf{L}_1^{-1}\mathbf{L}_2\mathbf{D}_2 & \text{is lower triangular} \end{array}$$

from which we conclude both sides, $\mathbf{D}_1\mathbf{U}_1\mathbf{U}_2^{-1}$ and $\mathbf{L}_1^{-1}\mathbf{L}_2\mathbf{D}_2$, are diagonal.

Proof

- Since both sides are diagonal, rearranging the equation shows the following

$$\mathbf{D}_1\mathbf{U}_1\mathbf{U}_2^{-1} = \mathbf{L}_1^{-1}\mathbf{L}_2\mathbf{D}_2 \implies \mathbf{U}_1\mathbf{U}_2^{-1} = \mathbf{D}_1^{-1}\mathbf{L}_1^{-1}\mathbf{L}_2\mathbf{D}_2$$

is also diagonal, and it has unit diagonals, thus

$$\mathbf{U}_1\mathbf{U}_2^{-1} = \mathbf{I}$$

since $\mathbf{U}_1$ and $\mathbf{U}_2^{-1}$ are upper triangular matrices with unit diagonals. Hence

$$\mathbf{U}_1 = \mathbf{U}_2$$

to avoid contradicting the inverse of a matrix is unique. Similarly,

$$\mathbf{L}_1 = \mathbf{L}_2$$

from which we conclude

$$\mathbf{D}_1 = \mathbf{D}_2 \quad \square$$

- Invoking the theorem $\boxed{15}$, if $\mathbf{A}$ can be reduced to an upper triangular matrix

$$\mathbf{U}$$

by using only Type III operations, then there exists a lower triangular matrix

$$\hat{\mathbf{L}}$$

with unit diagonals such that

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{U}$$

- Since we can always factor $\mathbf{U}$ into

$$\mathbf{U} = \mathbf{D}\hat{\mathbf{U}}$$

where $\mathbf{D}$ is diagonal and $\hat{\mathbf{U}}$ is upper triangular with unit diagonals, we have

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{D}\hat{\mathbf{U}}$$

- If $\mathbf{A}$ is invertible, then the last theorem says matrices on the right are unique

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{D}\hat{\mathbf{U}}$$

- Hence combining the last two theorems, we conclude the LU decomposition

$$\mathbf{A} = \hat{\mathbf{L}}\left(\mathbf{D}\hat{\mathbf{U}}\right) = \hat{\mathbf{L}}\mathbf{U}$$

  LU from Doolittle algorithm, when applicable, is unique if $\mathbf{A}$ is invertible.

- To see why LU is not necessarily unique for singular matrices, consider

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & x & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

  the rows of zeros in $\mathrm{rref}\left(\mathbf{A}\right)$ meant there are open choices for $\mathbf{L}$.

Q: Why being invertible is not sufficient to guarantee the existence of LU?

- Consider the following invertible matrix

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

- Assume there exists an LU decomposition for this matrix

$$\mathbf{A} = \mathbf{LU}$$

then either ℓ_{11} or u_{11} is zero since $a_{11} = 0$ and

$$a_{11} = \ell_{11} u_{11}$$

which means either $\mathbf{L}$ or $\mathbf{U}$ is singular, thus $\mathbf{A}$ is also singular.

- This contradicts to the fact that $\mathbf{A}$ is invertible

$$\det(\mathbf{A}) = -1$$

- Therefore, we conclude there is no LU decomposition for $\mathbf{A}$.

Definition

Suppose $\mathbf{A} \in \mathbb{R}^{n\times n}$, the kth order leading principal submatrix of $\mathbf{A}$, denoted by

$$\mathbf{A}_k$$

is the $k \times k$ submatrix of $\mathbf{A}$ at the upper-left corner of $\mathbf{A}$, that is,

$$\mathbf{A}_k = \mathbf{A}_{k\times k}$$

where $\mathbf{A}_{k\times k}$ is the submatrix if we partition $\mathbf{A} = \left[\begin{array}{c|c} \mathbf{A}_{k\times k} & \mathbf{B}_{k\times(n-k)} \\ \hline \mathbf{C}_{(n-k)\times k} & \mathbf{D}_{(n-k)\times(n-k)} \end{array}\right]$.

Theorem

Suppose $\mathbf{A}$ is an invertible $n \times n$ matrix. The leading principal submatrices $\mathbf{A}_k$ of $\mathbf{A}$ are invertible for $k = 1, \ldots, n-1$ if and only if $\mathbf{A}$ has the decomposition

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{U}$$

where $\hat{\mathbf{L}}$ is a unit lower triangular matrix and $\mathbf{U}$ is an upper triangular matrix.

Proof

- We use induction to show if the leading principal submatrices are invertible

$$\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_{n-1}$$

then the $\hat{\mathbf{L}}\mathbf{U}$ decomposition exists for an invertible matrix $\mathbf{A}$. It is clear that

$$\mathbf{A}_1 = \hat{\mathbf{L}}_1\mathbf{U}_1 = [1][a_{11}]$$

has such decomposition. Suppose $\mathbf{A}_{k-1}$ also has such decomposition

$$\mathbf{A}_{k-1} = \hat{\mathbf{L}}_{k-1}\mathbf{U}_{k-1}$$

and $\mathbf{A}_1$, $\cdots$, $\mathbf{A}_{k-1}$ are invertible. Consider the following partition of

$$\mathbf{A}_k = \left[\begin{array}{c:c} \mathbf{A}_{k-1} & \mathbf{B}_{(k-1)\times 1} \\ \hdashline \mathbf{C}_{1\times(k-1)} & a_{kk} \end{array}\right] = \underbrace{\left[\begin{array}{c:c} \hat{\mathbf{L}}_{k-1} & \mathbf{0}_{(k-1)\times 1} \\ \hdashline \mathbf{X} & 1 \end{array}\right]}_{\hat{\mathbf{L}}_k} \underbrace{\left[\begin{array}{c:c} \mathbf{U}_{k-1} & \mathbf{Y} \\ \hdashline \mathbf{0}_{1\times(k-1)} & u_{kk} \end{array}\right]}_{\mathbf{U}_k}$$

Proof

- If there is a choice for each of $\mathbf{X}$, $\mathbf{Y}$ and u_{kk}, then the decomposition exists

$$\left[\begin{array}{c:c} \mathbf{A}_{k-1} & \mathbf{B}_{(k-1)\times 1} \\ \hdashline \mathbf{C}_{1\times(k-1)} & a_{kk} \end{array}\right] = \underbrace{\left[\begin{array}{c:c} \hat{\mathbf{L}}_{k-1} & \mathbf{0}_{(k-1)\times 1} \\ \hdashline \mathbf{X} & 1 \end{array}\right]}_{\hat{\mathbf{L}}_k} \underbrace{\left[\begin{array}{c:c} \mathbf{U}_{k-1} & \mathbf{Y} \\ \hdashline \mathbf{0}_{1\times(k-1)} & u_{kk} \end{array}\right]}_{\mathbf{U}_k}$$

- Equating blocks, we have

$$\begin{aligned} \mathbf{X}\mathbf{U}_{k-1} + 1\cdot\mathbf{0}_{1\times(k-1)} = \mathbf{C}_{1\times(k-1)} \quad &\Longrightarrow \quad \mathbf{X} = \mathbf{C}_{1\times(k-1)}\mathbf{U}_{k-1}^{-1} \\ \hat{\mathbf{L}}_{k-1}\mathbf{Y} + \mathbf{0}_{(k-1)\times 1}u_{kk} = \mathbf{B}_{(k-1)\times 1} \quad &\Longrightarrow \quad \mathbf{Y} = \hat{\mathbf{L}}_{k-1}^{-1}\mathbf{B}_{(k-1)\times 1} \\ \mathbf{X}\mathbf{Y} + 1\cdot u_{kk} = a_{kk} \quad &\Longrightarrow \quad u_{kk} = a_{kk} - \mathbf{X}\mathbf{Y} \end{aligned}$$

- Since $\mathbf{A}_{k-1}$ is invertible, both of $\hat{\mathbf{L}}_{k-1}^{-1}$ and $\mathbf{U}_{k-1}^{-1}$ exist, hence

$$\hat{\mathbf{L}}_k \qquad \text{and} \qquad \mathbf{U}_k$$

exist and the decomposition $\mathbf{A} = \hat{\mathbf{L}}\mathbf{U}$ exists by the principle of induction.

Proof

- Conversely, if the decomposition exists

$$\mathbf{A} = \hat{\mathbf{L}}\mathbf{U}$$

- For $k = 1, \ldots, n-1$, the following partitions reveals $\mathbf{A}_k = \hat{\mathbf{L}}_k \mathbf{U}_k$

$$\mathbf{A} = \left[\begin{array}{c:c} \mathbf{A}_k & * \\ \hdashline * & * \end{array}\right] = \underbrace{\left[\begin{array}{c:c} \hat{\mathbf{L}}_k & \mathbf{0} \\ \hdashline * & * \end{array}\right]}_{\hat{\mathbf{L}}} \underbrace{\left[\begin{array}{c:c} \mathbf{U}_k & * \\ \hdashline \mathbf{0} & * \end{array}\right]}_{\mathbf{U}}$$

where $\mathbf{A}_k$, $\hat{\mathbf{L}}_k$ and $\mathbf{U}_k$ are the kth order leading principal submatrices of

$$\mathbf{A}, \qquad \hat{\mathbf{L}} \qquad \text{and} \qquad \mathbf{U}$$

respectively. Since $\mathbf{A}$ is invertible, $\hat{\mathbf{L}}$ and $\mathbf{U}$ have nonzero diagonals. So

$$\hat{\mathbf{L}}_k \qquad \text{and} \qquad \mathbf{U}_k$$

are invertible, which shows $\mathbf{A}_k = \hat{\mathbf{L}}_k \mathbf{U}_k$ is invertible for $k = 1, \ldots, n-1$ □

Q: How to adapt the $\hat{\mathbf{L}}\mathbf{U}$ decomposition to handle

$$\mathbf{A}$$

for which row interchanges are necessary during Gaussian elimination?

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 3 \\ 4 & 2 & 1 \\ 6 & -3 & 4 \end{bmatrix} = \mathbf{E}_{(2)1,2}\mathbf{E}_{(3)1,3}\mathbf{E}_{2,3}\mathbf{U}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -6 & -5 \\ 0 & 0 & -5 \end{bmatrix}$$

- Note the above matrix is invertible, but

$$\det(\mathbf{A}_2) = 0$$

whereas the related matrix $\tilde{\mathbf{A}} = \mathbf{E}_{2,3}\mathbf{A}$ has

$$\det\left(\tilde{\mathbf{A}}_1\right) = 2, \qquad \det\left(\tilde{\mathbf{A}}_2\right) = -12 \qquad \text{and} \qquad \det\left(\tilde{\mathbf{A}}_3\right) = 60$$

- Hence we could use Doolittle algorithm on $\tilde{\mathbf{A}}$ instead

$$
\begin{aligned}
\mathbf{A} = \mathbf{E}_{2,3}\mathbf{E}_{2,3}\mathbf{A} = \mathbf{E}_{2,3}\tilde{\mathbf{A}} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 6 & -3 & 4 \\ 4 & 2 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 3 \\ 0 & -6 & -5 \\ 0 & 0 & -5 \end{bmatrix}
\end{aligned}
$$

- Notice in this case only a single row interchange is needed,

$$\mathbf{E}_{i,j}$$

in general, we need a matrix that captures all the necessary row interchanges.

Definition

A permutation matrix, often denoted by $\mathbf{P}$, is a product of elementary matrices corresponding to row interchanges

- Note a permutation matrix is an identity matrix with rows being rearranged.

Theorem

If $\mathbf{P}$ is a permutation matrix, then $\mathbf{P}^{-1} = \mathbf{P}^{\mathrm{T}}$.

Proof

- Since the ith row of $\mathbf{P}$ corresponds to some standard unit row vector

$$\mathbf{e}_k^{\mathrm{T}}$$

whereas the jth column of $\mathbf{P}^{\mathrm{T}}$ also leads a standard unit column vector

$$\mathbf{e}_\ell$$

- Hence $\mathbf{P}\mathbf{P}^{\mathrm{T}}$ is an identity matrix, since $i = j$ if and only if $k = \ell$,

$$\left[\mathbf{P}\mathbf{P}^{\mathrm{T}}\right]_{ij} = \delta_{ij}$$

where δ_{ij} is the Kronecker delta. □

Theorem

Every invertible matrix $\mathbf{A}$ has a decomposition of the form

$$\mathbf{A} = \mathbf{P}^{\mathrm{T}}\hat{\mathbf{L}}\mathbf{U}$$

where $\mathbf{P}$ is a permutation matrix, $\hat{\mathbf{L}}$ is unit lower triangular, $\mathbf{U}$ is upper triangular.

Proof

- Since we need to show it is true for any $n \times n$ matrix, we use induction on n
- The claim is clearly true for $n = 1$,

$$[a_{11}] = [1]^{\mathrm{T}} [1] [a_{11}]$$

- Now suppose it is true for $n = k - 1$, and consider an invertible matrix

$$\mathbf{A}_{k \times k}$$

- Since $\mathbf{A}$ is invertible, one element in column one, say a_{r1}, must be nonzero.

Proof

- Let $\mathbf{B} = \mathbf{E}_{r,1}\mathbf{A}$, which has a nonzero element $b_{11} = a_{r1} \neq 0,$ and consider

$$\mathbf{M} = \mathbf{I} - \mathbf{c}\mathbf{e}_1^{\mathrm{T}} \qquad \text{where} \quad \mathbf{c} = \frac{1}{b_{11}} \begin{bmatrix} 0 \\ b_{21} \\ \vdots \\ b_{n1} \end{bmatrix} = \begin{bmatrix} 0 \\ \hline \mathbf{c}_{-1} \end{bmatrix}$$

- Notice $\mathbf{M}$ is unit lower triangular and thus invertible, and

$$\begin{aligned} \left(\mathbf{I} - \mathbf{c}\mathbf{e}_1^{\mathrm{T}}\right)\left(\mathbf{I} + \mathbf{c}\mathbf{e}_1^{\mathrm{T}}\right) &= \mathbf{I} - \mathbf{c}\mathbf{e}_1^{\mathrm{T}} + \mathbf{c}\mathbf{e}_1^{\mathrm{T}} - \mathbf{c}\mathbf{e}_1^{\mathrm{T}}\mathbf{c}\mathbf{e}_1^{\mathrm{T}} \\ &= \mathbf{I} - \mathbf{c}\left([0]_{1\times 1}\right)\mathbf{e}_1^{\mathrm{T}} \\ &= \mathbf{I} \\ \implies \mathbf{M}^{-1} &= \mathbf{I} + \mathbf{c}\mathbf{e}_1^{\mathrm{T}} \end{aligned}$$

- Direct computing the following, we see the first column of $\mathbf{MB}$ is

$$\mathbf{MBe}_1 = \mathbf{Be}_1 - \mathbf{c}\mathbf{e}_1^{\mathrm{T}}\mathbf{Be}_1 = \mathbf{Be}_1 - b_{11}\mathbf{c} = \begin{bmatrix} b_{11} & 0 & \cdots & 0 \end{bmatrix}^{\mathrm{T}}$$

Proof

- Consider the following partition of $\mathbf{MB}$,

$$\mathbf{MB} = \left[\begin{array}{c|c} b_{11} & \mathbf{F}_{1\times(k-1)} \\ \hline \mathbf{0}_{(k-1)\times 1} & \mathbf{G}_{(k-1)\times(k-1)} \end{array}\right]$$

- Recall $\mathbf{A}$ and $\mathbf{M}$ are invertible, and $\mathbf{E}_{r,1}$ is clearly invertible, consequently

$$\mathbf{MB} = \mathbf{ME}_{r,1}\mathbf{A}$$

is invertible as well, thus using the cofactor expansion

$$\det(\mathbf{MB}) = b_{11}\det(\mathbf{G}) \neq 0$$

we conclude $\mathbf{G}$ is also invertible. Hence by the induction hypothesis we have

$$\mathbf{G} = \mathbf{P}_G^{\mathrm{T}}\hat{\mathbf{L}}_G\mathbf{U}_G \implies \mathbf{P}_G\mathbf{G} = \hat{\mathbf{L}}_G\mathbf{U}_G$$

where $\mathbf{P}_G \in \mathbb{R}^{(k-1)\times(k-1)}$ is a permutation matrix, $\hat{\mathbf{L}}_G \in \mathbb{R}^{(k-1)\times(k-1)}$ is unit lower triangular, and $\mathbf{U} \in \mathbb{R}^{(k-1)\times(k-1)}$ is upper triangular.

Proof

- Let $\mathbf{Q} = \left[\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{P}_G^{\mathrm{T}} \end{array}\right]$, $\mathbf{N} = \left[\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0} & \hat{\mathbf{L}}_G \end{array}\right]$ and $\mathbf{U} = \left[\begin{array}{c|c} b_{11} & \mathbf{F} \\ \hline \mathbf{0} & \mathbf{U}_G \end{array}\right]$, then

$$\begin{aligned} \mathbf{Q}^{\mathrm{T}}\mathbf{M}\mathbf{E}_{r,1}\mathbf{A} = \mathbf{Q}^{\mathrm{T}}\mathbf{M}\mathbf{B} &= \left[\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{P}_G \end{array}\right] \left[\begin{array}{c|c} b_{11} & \mathbf{F} \\ \hline \mathbf{0} & \mathbf{G} \end{array}\right] \\ &= \left[\begin{array}{c|c} b_{11} & \mathbf{F} \\ \hline \mathbf{0} & \mathbf{P}_G\mathbf{G} \end{array}\right] \\ &= \left[\begin{array}{c|c} b_{11} & \mathbf{F} \\ \hline \mathbf{0} & \hat{\mathbf{L}}_G\mathbf{U}_G \end{array}\right] \\ &= \left[\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0} & \hat{\mathbf{L}}_G \end{array}\right] \left[\begin{array}{c|c} b_{11} & \mathbf{F} \\ \hline \mathbf{0} & \mathbf{U}_G \end{array}\right] = \mathbf{N}\mathbf{U} \end{aligned}$$

- Notice $\mathbf{Q}$ is a permutation matrix, and $\mathbf{E}_{r,1}^{-1} = \mathbf{E}_{r,1}$, thus

$$\mathbf{E}_{r,1}\mathbf{A} = \mathbf{M}^{-1}\mathbf{Q}\mathbf{N}\mathbf{U} \implies \mathbf{Q}^{\mathrm{T}}\mathbf{E}_{r,1}\mathbf{A} = \mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q}\mathbf{N}\mathbf{U}$$

where $\mathbf{P} = \mathbf{Q}^{\mathrm{T}}\mathbf{E}_{r,1}$ is a permutation matrix, and $\mathbf{U}$ is upper triangular.

Proof

- Hence the only thing left is to show $\mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q}\mathbf{N}$ is unit lower triangular.
- Considering $\mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q}$ explicitly,

$$
\begin{aligned}
\mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q} &= \mathbf{Q}^{\mathrm{T}}\left(\mathbf{I}+\mathbf{c}\mathbf{e}_1^{\mathrm{T}}\right)\mathbf{Q} \\
&= \mathbf{I}+\mathbf{Q}^{\mathrm{T}}\mathbf{c}\mathbf{e}_1^{\mathrm{T}}\mathbf{Q} \\
&= \mathbf{I}+\left[\begin{array}{c:c} 1 & \mathbf{0} \\ \hdashline \mathbf{0} & \mathbf{P}_G \end{array}\right]\left[\begin{array}{c:c} 0 & \\ \hdashline b_{21}/b_{11} & \\ \vdots & \mathbf{0}_{k\times(k-1)} \\ b_{n1}/b_{11} & \end{array}\right]\left[\begin{array}{c:c} 1 & \mathbf{0} \\ \hdashline \mathbf{0} & \mathbf{P}_G^{\mathrm{T}} \end{array}\right] \\
&= \mathbf{I}+\left[\begin{array}{c:c} 0 & \\ \hdashline \mathbf{P}_G\mathbf{c}_{-1} & \mathbf{0}_{k\times(k-1)} \end{array}\right]\left[\begin{array}{c:c} 1 & \mathbf{0} \\ \hdashline \mathbf{0} & \mathbf{P}_G^{\mathrm{T}} \end{array}\right] \\
&= \mathbf{I}+\left[\begin{array}{c:c} 0 & \\ \hdashline \mathbf{P}_G\mathbf{c}_{-1} & \mathbf{0}_{k\times(k-1)} \end{array}\right]
\end{aligned}
$$

- Clearly $\mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q}$ is unit lower triangular, so $\hat{\mathbf{L}}=\mathbf{Q}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{Q}\mathbf{N}$ is unit lower triangular since $\mathbf{N}$ is unit lower triangular, which completes the proof. □

Matlab

Command Window

```
>>
>> A = [ 0 0 6; 1 2 3; 2 1 4]

A =

     0     0     6
     1     2     3
     2     1     4

>> n = size(A,1);
>> % You need to modify it slightly to have the output
>> GaussianElimination(A,zeros(n,1));
Row 1 is interchanged with row 2
Row 2 is interchanged with row 3
>> P = [0 0 1; 0 1 0; 1 0 0]

P =

     0     0     1
     0     1     0
     1     0     0

>> GaussianElimination(P*A,zeros(n,1));
>> % No interchange no output
>> Atilde = P*A

Atilde =

     2     1     4
     1     2     3
     0     0     6

>>
```

Command Window

```
>>
>> [L, U] = ludecomp(Atilde);
>> transpose(P)*L*U

ans =

     0     0     6
     1     2     3
     2     1     4

>> [L, U, P] = lu(A)

L =

    1.0000         0         0
    0.5000    1.0000         0
         0         0    1.0000


U =

    2.0000    1.0000    4.0000
         0    1.5000    1.0000
         0         0    6.0000


P =

     0     0     1
     0     1     0
     1     0     0

>>
```