## Numerical Methods



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## Linear Systems

This chapter deals with simultaneous linear algebraic equations that can be represented generally as

$$
\begin{array}{cc}
E_{1}: & a_{11} x_{1}+a_{12} x_{2}+\cdots+a_{1 n} x_{n}=b_{1}, \\
E_{2}: & a_{21} x_{1}+a_{22} x_{2}+\cdots+a_{2 n} x_{n}=b_{2} \\
& \vdots \\
E_{n}: & a_{n 1} x_{1}+a_{n 2} x_{2}+\cdots+a_{n n} x_{n}=b_{n},
\end{array}
$$

### 1.0.1 The graphical method

A graphical solution is obtainable for two equations by plotting them on Cartesian coordinates with one axis corresponding to $x_{1}$ and the other to $x_{2}$.

$$
\begin{align*}
& a_{11} x_{1}+a_{12} x_{2}=b_{1}  \tag{1.1}\\
& a_{21} x_{1}+a_{22} x_{2}=b_{2} \tag{1.2}
\end{align*}
$$

Both equations can be solved for $x_{2}$ :

$$
\begin{align*}
& x_{2}=-\left(\frac{a_{11}}{a_{12}}\right) x_{1}+\frac{b_{1}}{a_{12}}  \tag{1.3}\\
& x_{2}=-\left(\frac{a_{21}}{a_{22}}\right) x_{1}+\frac{b_{2}}{a_{22}} \tag{1.4}
\end{align*}
$$

## 1. LINEAR SYSTEMS

Thus, the equations are now in the form of straight lines; that is, $x_{2}=$ (slope) $x_{1}+$ intercept. These lines can be graphed on Cartesian coordinates with $x_{2}$ as the ordinate and $x_{1}$ as the abscissa. The values of $x_{1}$ and $x_{2}$ at the intersection of the lines represent the solution.

## Example

$$
\begin{align*}
3 x_{1}+2 x_{2} & =18  \tag{1.5}\\
-x_{1}+2 x_{2} & =2 \tag{1.6}
\end{align*}
$$



For three simultaneous equations, each equation would be represented by a plane in a threedimensional coordinate system. The point where the three planes intersect would represent the solution.

By a sequence of operation, a linear system can be transformed to a more easily solved linear system that has the same solutions.

$$
\begin{aligned}
& \begin{array}{rlrlll}
E_{1} & : & x_{1} & + & x_{2} & +3 x_{4} \\
E_{2} & : & x_{1} & + & x_{2} & -\quad x_{3} \\
+ & x_{4} & =1,
\end{array} \\
& E_{3}: 3 x_{1}-x_{2}-x_{3}+2 x_{4}=-3 \\
& E_{4}:-x_{1}+2 x_{2}+3 x_{3}-x_{4}=4 \text {, }
\end{aligned}
$$

will be solved for $x_{1}, x_{2}, x_{3}$ and $x_{4}$. We use $E_{1}$ to eliminate the unknown $x_{1}$ from $E_{2}, E_{3}$ and $E_{4}$ by performing $\left(E_{2}-2 E_{1}\right) \rightarrow\left(E_{2}\right),\left(E_{3}-3 E_{1}\right) \rightarrow\left(E_{3}\right)$ and $\left(E_{4}+E_{1}\right) \rightarrow\left(E_{4}\right)$. The resulting system is

$$
\begin{array}{rlllrlllll}
E_{1} & : & x_{1} & + & x_{2} & & & + & 3 x_{4} & =4, \\
E_{2} & : & & - & x_{2} & - & x_{3} & - & 5 x_{4} & =-7, \\
E_{3} & : & & - & 4 x_{2} & - & x_{3} & - & 7 x_{4} & =-15 \\
E_{4} & : & & + & 3 x_{2} & + & 3 x_{3} & + & 2 x_{4} & =8,
\end{array}
$$

In the new system, $E_{2}$ is used to eliminate $x_{2}$ from $E_{3}$ and $E_{4}$ by performing $\left(E_{3}=4 E_{2}\right) \rightarrow$ $\left(E_{3}\right)$ and $\left(E_{4}+3 E_{2}\right) \rightarrow\left(E_{4}\right)$

| $E_{1}$ | $:$ | $x_{1}$ | + | $x_{2}$ |  |  | + | $3 x_{4}$ | $=4$, |
| ---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $E_{2}$ | $:$ |  | - | $x_{2}$ | - | $x_{3}$ | - | $5 x_{4}$ | $=$ |
| $E_{3}$ | $:$ |  |  |  |  | $3 x_{3}$ | + | $13 x_{4}$ | $=13$ |
| $E_{4}$ | $:$ |  |  |  |  |  | - | $13 x_{4}$ | $=$ |

The system of equations is now in triangular (or reduced) form and can be solved for the unknowns by a backward-substitution process. The solution is therefore $x_{4}=-1, x_{2}=$ $2, x_{3}=0$ and $x_{4}=1$.

The only variation from system to system occurred in the coefficients of the unknowns and in the values on the right side. For this reason, a linear system is often replaced by a matrix.

Definition: An $\boldsymbol{n} \times \boldsymbol{m}$ matrix is a rectangular array of elements with $\boldsymbol{n}$ rows and $\boldsymbol{m}$ columns.

The notation for an $n \times m$ matrix will be capital letter such as $A$ for the matrix and lowercase letter with double subscripts, such as $a_{i j}$ to refer to the entry at the intersection of the $i$ th row and $j$ th columns.

$$
A=a_{i j}=\left[\begin{array}{cccc}
a_{11} & a_{12} & \cdots & a_{1 m} \\
a_{21} & a_{22} & \cdots & a_{2 m} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n 1} & a_{n 2} & \cdots & a_{n m}
\end{array}\right]
$$

The $1 \times n$ matrix

$$
A=\left[\begin{array}{llll}
a_{11} & a_{12} & \cdots & a_{1 n}
\end{array}\right]
$$

is called an $\mathbf{n}$-dimensional row vector, and an $n \times 1$ matrix

$$
A=\left[\begin{array}{c}
a_{11} \\
a_{21} \\
\vdots \\
a_{n 1}
\end{array}\right]
$$

is called an $\mathbf{n}$-dimensional column vector.

An $n \times(n+1)$ matrix can be used to represent the linear system

$$
\begin{align*}
a_{11} x_{1}+a_{12} x_{2}+\cdots+a_{1 n} x_{n} & =b_{1}  \tag{1.7}\\
a_{21} x_{1}+a_{22} x_{2}+\cdots+a_{2 n} x_{n} & =b_{2}  \tag{1.8}\\
\vdots & \vdots  \tag{1.9}\\
a_{n 1} x_{1}+a_{n 2} x_{2}+\cdots+a_{n n} x_{n} & =b_{n} \tag{1.10}
\end{align*}
$$

by first constructing

$$
A=\left[\begin{array}{cccc}
a_{11} & a_{12} & \cdots & a_{1 m} \\
a_{21} & a_{22} & \cdots & a_{2 m} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n 1} & a_{n 2} & \cdots & a_{n m}
\end{array}\right] \quad \text { and } \quad b=\left[\begin{array}{c}
b_{1} \\
b_{2} \\
\vdots \\
b_{n}
\end{array}\right]
$$

and then combining these matrices to form the augmented matrix

$$
[A, b]=\left[\begin{array}{cccccc}
a_{11} & a_{12} & \cdots & a_{1 m} & \vdots & b_{1} \\
a_{21} & a_{22} & \cdots & a_{2 m} & \vdots & b_{2} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
a_{n 1} & a_{n 2} & \cdots & a_{n m} & \vdots & b_{n}
\end{array}\right]
$$

So the matrix in the example:

$$
\left[\begin{array}{cccccc}
1 & 1 & 0 & 3 & \vdots & 4 \\
2 & 1 & -1 & 1 & \vdots & 1 \\
3 & -1 & -1 & 2 & \vdots & -3 \\
-2 & 2 & 3 & -2 & \vdots & 4
\end{array}\right] \rightarrow\left[\begin{array}{cccccc}
1 & 1 & 0 & 3 & \vdots & 4 \\
0 & -1 & -1 & -5 & \vdots & -7 \\
0 & 0 & 3 & 13 & \vdots & 13 \\
0 & 0 & 0 & -13 & \vdots & -13
\end{array}\right]
$$

The procedure involved is called Gaussian elimination with backward substitution.

The general Gaussian procedure: first form the augmented matrix $\tilde{A}$

$$
\tilde{A}=\left[\begin{array}{cccccc}
a_{11} & a_{12} & \cdots & a_{1 n} & \vdots & a_{1, n+1} \\
a_{21} & a_{22} & \cdots & a_{2 n} & \vdots & a_{2, n+1} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
a_{n 1} & a_{n 2} & \cdots & a_{n n} & \vdots & a_{n, n+1}
\end{array}\right]
$$

Provided $a_{11} \neq 0$, the operations corresponding to $\left(E_{j}-\left(a_{j 1} / a_{11}\right) E_{1}\right) \rightarrow\left(E_{j}\right)$ are performed for each $j=2,3, \cdots, n$ to eliminate the coefficient of $x_{1}$ in each of these rows. With this in mind, we follow the sequential procedure for $i=2,3, \cdots, n$ and perform the operation $\left(E_{j}-\left(a_{j i} / a_{i i}\right) E_{i}\right) \rightarrow\left(E_{j}\right)$ for each $j=i+1, i+2, \cdots, n$.
The resulting matrix has the form

$$
\tilde{\tilde{A}}=\left[\begin{array}{cccccc}
a_{11} & a_{12} & \cdots & a_{1 n} & \vdots & a_{1, n+1} \\
0 & a_{22} & \cdots & a_{2 n} & \vdots & a_{2, n+1} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & \cdots & \cdots 0 & a_{n n} & \vdots & a_{n, n+1}
\end{array}\right]
$$

where the values of $a_{i j}$ are not expected to agree with those in the original matrix $\tilde{A}$. For these linear system, a backward substitution can be performed. Solving the $n$th equation for $x_{n}$ gives

$$
x_{n}=\frac{a_{n, n+1}}{a_{n n}}
$$

Solving the $(n-1)$ st equation for $x_{n-1}$ and using $x_{n}$ yields

$$
x_{n-1}=\frac{a_{n-1, n+1}-a_{n-1, n} x_{n}}{a_{n-1, n-1}}
$$

Continuing this process, we obtain

$$
x_{i}=\frac{a_{i, n+1}-a_{i, n} x_{n}-a_{i, n-1} x_{n-1}-\cdots-a_{i, i+1} x_{i+1}}{a_{i i}}=\frac{a_{i, n+1}-\sum_{j=i+1}^{n} a_{i j} x_{j}}{a_{i i}}
$$

for each $i=n-1, n-2, \cdots, 2,1$.
The Gaussian elimination procedure can be presented more precisely

The procedure will fail if one of the elements $a_{11}^{(1)}, a_{22}^{(2)}, a_{33}^{(3)}, \cdots, a_{n-1, n-1}^{(n-1)}, a_{n n}^{(n)}$ is zero because the step

$$
\left(E_{i}-\frac{a_{i, k}^{(k)}}{a_{k k}^{(k)}} E_{k}\right) \rightarrow E_{i}
$$

cannot be performed.
$a_{i j}^{(k)}= \begin{cases}a_{i j}^{(k-1)}, & \text { when } i=1,2, \ldots, k-1 \text { and } j=1,2, \ldots, n+1, \\ 0, & \text { when } i=k, k+1, \ldots, n \text { and } j=1,2, \ldots, k-1, \\ a_{i j}^{(k-1)}-\frac{a_{i, k-1}^{(k-1)}}{a_{k-1, k-1}^{(k-1)}} a_{k-1, j}^{(k-1)}, & \text { when } i=k, k+1, \ldots, n \text { and } j=k, k+1, \ldots, n+1 .\end{cases}$
$\tilde{A}^{(k)}=\left[\begin{array}{cccccccc:c}a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1, k-1}^{(1)} & a_{1 k}^{(1)} & \cdots & a_{1 n}^{(1)} & a_{1, n+1}^{(1)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & \cdots & a_{2, k-1}^{(2)} & a_{2 k}^{(2)} & \cdots & a_{2 n}^{(2)} & a_{2, n+1}^{(2)} \\ \vdots & \ddots & \ddots & & \vdots & \vdots & & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & a_{k-1, k-1}^{(k-1)} & a_{k-1, k}^{(k-1)} & \cdots & a_{k-1, n}^{(k-1)} & a_{k-1, n+1}^{(k-1)} \\ \vdots & & & 0 & a_{k k}^{(k)} & \cdots & a_{k n}^{(k)} & a_{k, n+1}^{(k)} \\ \vdots & & & \vdots & \vdots & & \vdots & \vdots \\ 0 & \cdots \cdots \cdots \cdots \cdots \cdots & 0 & a_{n k}^{(k)} & \cdots & a_{n n}^{(k)} & a_{n, n+1}^{(k)}\end{array}\right]$

## Example:

$$
\begin{array}{rcrcccccccl}
E_{1} & : & x_{1} & - & x_{2} & + & 2 x_{3} & - & x_{4} & = & -8, \\
E_{2} & : & 2 x_{1} & - & 2 x_{2} & - & 3 x_{3} & - & 3 x_{4} & = & -20, \\
E_{3} & : & x_{1} & + & x_{2} & + & x_{3} & & & = & -2, \\
E_{4} & : & x_{1} & - & x_{2} & + & 4 x_{3} & + & 3 x_{4} & = & 4, \\
& \tilde{A}=\tilde{A}^{(1)}=\left[\begin{array}{cccccc}
1 & -1 & 2 & -1 & \vdots & -8 \\
2 & -2 & 3 & -3 & \vdots & -20 \\
1 & 1 & 1 & 0 & \vdots & -2 \\
1 & -2 & 4 & 3 & \vdots & 4
\end{array}\right]
\end{array}
$$

and performing the operations

$$
\left(E_{2}-2 E_{1}\right) \rightarrow\left(E_{2}\right),\left(E_{3}-E_{1}\right) \rightarrow\left(E_{3}\right), \quad \text { and } \quad\left(E_{4}-E_{1}\right) \rightarrow\left(E_{4}\right)
$$

gives

$$
\tilde{A}^{(2)}=\left[\begin{array}{cccccc}
1 & -1 & 2 & -1 & \vdots & -8 \\
0 & 0 & -1 & -1 & \vdots & -4 \\
0 & 2 & -1 & 1 & \vdots & 6 \\
0 & 0 & 2 & 4 & \vdots & 12
\end{array}\right]
$$

Since $a_{22}^{(2)}$, called the pivot element, is zero, the procedure cannot continue in its present form. Since $a_{32}^{(2)} \neq 0$, the operation $\left(E_{2}\right) \leftrightarrow\left(E_{3}\right)$ is performed to obtain a new matrix

$$
\tilde{A}^{(2)^{\prime}}=\left[\begin{array}{cccccc}
1 & -1 & 2 & -1 & \vdots & -8 \\
0 & 2 & -1 & 1 & \vdots & 6 \\
0 & 0 & -1 & -1 & \vdots & -4 \\
0 & 0 & 2 & 4 & \vdots & 12
\end{array}\right]
$$

$\tilde{A}^{(3)}$ will be $\tilde{A}^{(2)^{\prime}}$, and the computations continue with the operation $\left(E_{4}+2 E_{3}\right) \rightarrow\left(E_{4}\right)$, giving

$$
\tilde{A}^{(2)^{\prime}}=\left[\begin{array}{cccccc}
1 & -1 & 2 & -1 & \vdots & -8 \\
0 & 2 & -1 & 1 & \vdots & 6 \\
0 & 0 & -1 & -1 & \vdots & -4 \\
0 & 0 & 0 & 2 & \vdots & 4
\end{array}\right]
$$

Finally, the backward substitution is applied

$$
\begin{align*}
& x_{4}=\frac{4}{2}=2  \tag{1.11}\\
& x_{3}=\frac{\left[-4-(-1) x_{4}\right]}{-1}=2  \tag{1.12}\\
& x_{2}=\frac{\left[6-x_{4}-(-1) x_{3}\right]}{2}=3  \tag{1.13}\\
& x_{1}=\frac{-8-(-1) x_{4}-2 x_{3}-(-1) x_{2}}{1}=-7 \tag{1.14}
\end{align*}
$$

If $a_{p k}^{(k)}=0$ for each $p$, it can be shown (Thm) that the linear system does not have a unique solution and the procedure stops.

The first system has an infinite number of solutions, and the second leads to a contradiction, hence no solution exists.
https://numpy.org/doc/stable/reference/routines.linalg.html https://docs.scipy.org/doc/scipy/reference/linalg.html
(hw: from a geometrical standpoint $x_{1}+2 x_{2}=3,2 x_{1}+4 x_{2}=6$. Using Gaussian elimination with backward sustitution: $4 x_{1}-x_{2}+x_{3}=8,2 x_{1}+5 x_{2}+2 x_{3}=3, x_{1}+2 x_{2}+4 x_{3}=11$. )

$$
\begin{array}{rlrl}
x_{1}+x_{2}+x_{3} & =4, \\
2 x_{1}+2 x_{2}+x_{3} & =6, \quad \text { and } \quad x_{1} \quad 2 x_{1}+2 x_{2}+x_{3} & =4 \\
x_{1}+x_{2}+2 x_{3} & =6, & & x_{1}+x_{2}+2 x_{3}
\end{array}=6,
$$

These systems produce matrices

$$
\tilde{A}=\left[\begin{array}{lllll}
1 & 1 & 1 & \vdots & 4 \\
2 & 2 & 1 & \vdots & 6 \\
1 & 1 & 2 & \vdots & 6
\end{array}\right] \text { and } \quad \tilde{A}=\left[\begin{array}{ccc:c}
1 & 1 & 1 & \vdots \\
2 & 2 & 1 & \vdots \\
1 & 1 & 2 & \vdots
\end{array}\right]
$$

Since $a_{11}=1$, we perform $\left(E_{2}-2 E_{1}\right) \rightarrow\left(E_{2}\right)$ and $\left(E_{3}-E_{1}\right) \rightarrow\left(E_{3}\right)$ to produce

$$
\tilde{A}=\left[\begin{array}{rrr:r}
1 & 1 & 1 & \vdots \\
0 & 0 & -1 & 4 \\
0 & 0 & 1 & -2 \\
2
\end{array}\right] \quad \text { and } \quad \tilde{A}=\left[\begin{array}{rrr:r}
1 & 1 & 1 & 4 \\
0 & 0 & -1 & -4 \\
0 & 0 & 1 & 2
\end{array}\right]
$$

At this point, $a_{22}=a_{32}=0$. The algorithm requires that the procedure be halted, and no solution to either system is obtained. Writing the equations for each system gives

$$
\begin{aligned}
& x_{1}+x_{2}+x_{3}=4, \quad x_{1}+x_{2}+x_{3}=4, \\
& -x_{3}=-2, \text { and } \quad-x_{3}=-4 \text {, } \\
& x_{3}=2, \quad x_{3}=2 .
\end{aligned}
$$

First we require $(n-i)$ divisions. The replacement of $E_{j}$ by $\left(E_{j}-m_{i j} E_{i}\right)$ requires $(n-i)(n-$ $i+1)$ multiplications. Then each term is subtracted, which requires $(n-i)(n-i+1)$ subtractions.

Multiplications/divisions

$$
(n-i)+(n-i)(n-i+1)=(n-i)(n-i+2)
$$

Additions/subtractions

$$
(n-i)(n-i+1)
$$

Multiplications/divisions

$$
\sum_{i=1}^{n-1}(n-i)(n-i+2)=\frac{2 n^{3}+3 n^{2}-5 n}{6}
$$

Additions/subtractions

$$
\sum_{i=1}^{n-1}(n-i)(n-i+1)=\frac{n^{3}-n}{3}
$$

For the backward substitution, requires $(n-i)$ multiplications and $(n-i-1)$ additions for each summation term, and one subtraction and one division.

Multiplications/divisions

$$
1+\sum_{i=1}^{n-1}((n-i)+1)=\frac{n^{2}+n}{2}
$$

Additions/subtractions

$$
\sum_{i=1}^{n-1}((n-i-1)+1)=\frac{n^{2}-n}{2}
$$

Giving a total number

## Multiplications/divisions

$$
\frac{2 n^{3}+3 n^{2}-5 n}{6}+\frac{n^{2}+n}{2}=\frac{n^{3}}{3}+n^{2}-\frac{n}{3}
$$

## Additions/subtractions

$$
\frac{n^{3}-n}{3}+\frac{n^{2}-n}{2}=\frac{n^{3}}{3}+\frac{n^{2}}{2}-\frac{5 n}{6}
$$

| $n$ | Multiplications/Divisions | Additions/Subtractions |
| ---: | :---: | :---: |
| 3 | 17 | 11 |
| 10 | 430 | 375 |
| 50 | 44,150 | 42,875 |
| 100 | 343,300 | 338,250 |

### 1.0.2 Gauss-Jordan

The GJ method requires: Multiplications/divisions

$$
\frac{n^{3}}{3}+\frac{3 n^{2}}{2}-\frac{5 n}{6}
$$

Additions/subtractions

$$
\frac{n^{3}}{2}-\frac{n}{2}
$$

(hw: make a table comparing the required operation for $n=3,10,50,100$. Which method requires less computation?)

$$
\left[\begin{array}{cccccc}
a_{11}^{(1)} & 0 & \cdots & 0 & \vdots & a_{1, n+1}^{(1)} \\
0 & a_{22}^{(2)} & \ddots & \vdots & \vdots & a_{2, n-1}^{(2)} \\
\vdots & \ddots & \ddots & 0 & \vdots & \vdots \\
0 & \cdots & 0 & a_{n n}^{(n)} & \vdots & a_{n, n+1}^{(n)}
\end{array}\right]
$$

(hw: solve:

$$
\begin{align*}
0.003000 x_{1}+59.14 x_{2} & =59.17  \tag{1.15}\\
5.291 x_{1}-6.130 x_{2} & =46.78 \tag{1.16}
\end{align*}
$$

)

$$
\begin{aligned}
\pi x_{1}-e x_{2}+\sqrt{2} x_{3}-\sqrt{3} x_{4} & =\sqrt{11} \\
\pi^{2} x_{1}+e x_{2}-e^{2} x_{3}+\frac{3}{7} x_{4} & =0 \\
\sqrt{5} x_{1}-\sqrt{6} x_{2}+x_{3}-\sqrt{2} x_{4} & =\pi \\
\pi^{3} x_{1}+e^{2} x_{2}-\sqrt{7} x_{3}+\frac{1}{9} x_{4} & =\sqrt{2} .
\end{aligned}
$$

Actual solution $(0.78839378,-3.12541367,0.16759660,4.55700252)^{t}$.

### 1.1 Pivoting Strategies

To reduce roundoff error, it is often necessary to perform row interchanges even when the pivot elements are not zero. If $a_{k k}^{(k)}$ is small in magnitude compared to $a_{j k}^{(k)}$, the magnitude of the multiplier

$$
m_{j k}=\frac{a_{j k}^{(k)}}{a_{k k}^{(k)}}
$$

will be much larger that 1 . Also, when performing the backward substitution.

The linear system

$$
\begin{align*}
0.003000 x_{1}+59.14 x_{2} & =59.17  \tag{1.17}\\
5.291 x_{1}-6.130 x_{2} & =46.78 \tag{1.18}
\end{align*}
$$

### 1.1 Pivoting Strategies

has exact solution $x_{1}=10.00$ and $x_{2}=1.000$. Performing $\left(E_{2}-m_{21} E_{1}\right) \rightarrow\left(E_{2}\right)$ and the appropriate rounding gives

$$
\begin{align*}
0.003000 x_{1}+59.14 x_{2} & =59.17  \tag{1.19}\\
-104300 x_{2} & =-104400 \tag{1.20}
\end{align*}
$$

The disparity in the magnitudes of $m_{21} a_{13}$ and $a_{23}$ has introduced roundoff error, but the roundoff error has not yet been propagated. Backward substitution yields

$$
x_{2}=1.001
$$

and

$$
x_{1} \equiv \frac{59.17-(59.14)(1.001)}{0.003000}=-10.00
$$

To avoid this problem, pivoting is performed by selecting a larger element $a_{p q}^{(k)}$ for the pivot and interchanging the $k$ th and $q$ th columns, if necessary. We determine the smallest $p \geq k$ such that

$$
\left|a_{p k}^{(k)}\right| \max _{k \leq i \leq n}\left|a_{i k}^{k}\right|
$$

and perform $\left(E_{k}\right) \leftrightarrow\left(E_{p}\right)$.
Consider the same example. The pivoting procedure just described results in first finding

$$
\max \left\{\left|a_{11}^{(1)}\right|,\left|a_{21}^{(1)}\right|\right\}=\max \{|0.003000| \cdot|5.291|\}=|5.291|=\left|a_{21}^{(1)}\right|
$$

The operation $\left(E_{2}\right) \leftrightarrow\left(E_{1}\right)$ is then performed to give the system

$$
\begin{align*}
5.291 x_{1}-6.130 x_{2} & =46.78  \tag{1.21}\\
0.003000 x_{1}+59.14 x_{2} & =59.17 \tag{1.22}
\end{align*}
$$

which reduces to

$$
\begin{align*}
5.291 x_{1}-6.130 x_{2} & =46.78  \tag{1.23}\\
59.14 x_{2} & =59.14 \tag{1.24}
\end{align*}
$$

The correct values $x_{1}=10.00$ and $x_{2}=1.000$. This technique is called partial pivoting or maximal column pivoting.

### 1.2 Linear Algebra and Matrix Inversion

Equal matrices, sum, multiplication by scalar, matrix product, transpose,
An upper-triangular $n \times n$ matrix $U=\left(u_{i j}\right)$ has, for each $j=1,2, \cdots, n$, the entries

$$
u_{i j}=0, \quad \text { for each } i=j+1, j+2, \cdots, n
$$

and a lower-triangular matrix $L=\left(l_{i j}\right)$ has, for each $j=1,2, \cdots, n$, the entries

$$
l_{i j}=0, \quad \text { for each } i=j+1, j+2, \cdots, n
$$

An $n \times n$ matrix $A$ is said to be nonsingular (or invertible) if an $n \times n$ matrix $A^{-1}$ exist with $A A^{-1}=A^{-1} A=I$. The matrix $A^{-1}$ is called the inverse of $A$.

If we have the inverse of $A$, we can easily solve a linear system of the form $A x=b$.

$$
\left[\begin{array}{ccc}
1 & 2 & -1 \\
2 & 1 & 0 \\
-2 & 1 & 2
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
2 \\
3 \\
4
\end{array}\right]
$$

and then multiply both sides by the inverse, gives the solution $x_{1}=7 / 9, x_{2}=13 / 9$ and $x_{3}=5 / 3$.
Even though it is easier to solve a linear system of the form $A x=b$ if $A^{-1}$ is known, it is not computationally efficient to determine $A^{-1}$ in order to solve the system.

To determine the inverse of the matrix

$$
\left[\begin{array}{ccc}
1 & 2 & -1 \\
2 & 1 & 0 \\
-2 & 1 & 2
\end{array}\right]
$$

let us first consider the product $A B$, where $B$ is an arbitrary $3 \times 3$ matrix.

$$
\begin{aligned}
A B & =\left[\begin{array}{rrr}
1 & 2 & -1 \\
2 & 1 & 0 \\
-1 & 1 & 2
\end{array}\right]\left[\begin{array}{lll}
b_{11} & b_{12} & b_{13} \\
b_{21} & b_{22} & b_{23} \\
b_{31} & b_{32} & b_{33}
\end{array}\right] \\
& =\left[\begin{array}{ccc}
b_{11}+2 b_{21}-b_{31} & b_{12}+2 b_{22}-b_{32} & b_{13}+2 b_{23}-b_{33} \\
2 b_{11}+b_{21} & 2 b_{12}+b_{22} & 2 b_{13}+b_{23} \\
-b_{11}+b_{21}+2 b_{31} & -b_{12}+b_{22}+2 b_{32} & -b_{13}+b_{23}+2 b_{33}
\end{array}\right]
\end{aligned}
$$

If $B=A^{-1}$, then $A B=I$, so we must have

$$
\begin{aligned}
b_{11}+2 b_{21}-b_{31} & =1, & b_{12}+2 b_{22}-b_{32} & =0, & b_{13}+2 b_{23}-b_{33} & =0, \\
2 b_{11}+b_{21} & =0, & 2 b_{12}+b_{22} & =1, & 2 b_{13}+b_{23} & =0 \\
-b_{11}+b_{21}+2 b_{31} & =0, & -b_{12}+b_{22}+2 b_{32} & =0, & -b_{13}+b_{23}+2 b_{33} & =1 .
\end{aligned}
$$

Notice that the coefficients in each of the systems of equations are the same, the only change in the systems occurs on the right side of the equations, therefore

$$
\left[\begin{array}{ccccccc}
1 & 2 & -1 & \vdots & 1 & 0 & 0 \\
2 & 1 & 0 & \vdots & 0 & 1 & 0 \\
-2 & 1 & 2 & \vdots & 0 & 0 & 1
\end{array}\right]
$$

First performing $\left(E_{2}-2 E_{1}\right) \rightarrow\left(E_{2}\right)$ and $\left(E_{3}+E_{1}\right) \rightarrow\left(E_{3}\right)$, followed by $\left(E_{3}+E_{2}\right) \rightarrow\left(E_{3}\right)$ produces

$$
\left[\begin{array}{ccccccc}
1 & 2 & -1 & \vdots & 1 & 0 & 0 \\
0 & -3 & 2 & \vdots & -2 & 1 & 0 \\
0 & 3 & 1 & \vdots & 1 & 0 & 1
\end{array}\right] \quad \text { and }\left[\begin{array}{ccccccc}
1 & 2 & -1 & \vdots & 1 & 0 & 0 \\
0 & -3 & 2 & \vdots & -2 & 1 & 0 \\
0 & 0 & 3 & \vdots & -1 & 1 & 1
\end{array}\right]
$$

Backward substitution gives (three systems of eqns.)

$$
A^{-1}=\left[\begin{array}{ccc}
-\frac{2}{9} & \frac{5}{9} & -\frac{1}{9} \\
\frac{4}{9} & -\frac{1}{9} & \frac{2}{9} \\
-\frac{1}{3} & \frac{1}{3} & \frac{1}{3}
\end{array}\right]
$$

As we saw in that example, it is convenient to set up a larger augmented matrix, $[A: I]$. Upon performing the elimination in accordance, we obtain an augmented matrix of the form $[U: L]$.

### 1.3 Matrix Factorization

The steps used to solve a system of the form $A x=b$ can be used to factor a matrix. The factorization is particularly useful when it has the form $A=L U$.
If $A$ has been factored into the triangular form $A=L U$, then we can solve for $x$ more easily by using a two-step process. First we let $y=U x$ and solve the system $L y=b$ for $y$. Since $L$ is triangular, determining $y$ from this equation requires only $\mathcal{O}\left(n^{2}\right)$ operations. Once $y$ is known, the upper triangular system $U x=y$ requires only an additional $\mathcal{O}\left(n^{2}\right)$ to determine the solution $x$. Then, the number of operations is reduced from $\mathcal{O}\left(n^{3}\right)$ to $\mathcal{O}\left(n^{2}\right)$.

If Gaussian elimination can be performed on the linear system $A \mathbf{x}=\mathrm{b}$ without row interchanges, then the matrix $A$ can be factored into the product of a lower-triangular matrix $L$ and an upper-triangular matrix $U$,

$$
A=L U,
$$

where $m_{j i}=a_{j i}^{(i)} / a_{i i}^{(i)}$,

$$
U=\left[\begin{array}{ccccc}
a_{11}^{(1)} & a_{12}^{(1)} & \cdots \cdots \cdots & a_{1 n}^{(1)} \\
0 & a_{22}^{(2)} & \ddots & \ddots & \vdots \\
\vdots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & a_{n-1, n}^{(n-1)} \\
0 & \cdots & \cdots & 0 & \\
a_{n n}^{(n)}
\end{array}\right], \quad \text { and } \quad L=\left[\begin{array}{ccccc}
1 & 0 & : & \cdots \cdots \cdots & 0 \\
m_{21} & 1 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & 0 \\
m_{n 1} & \cdots & m_{n, n-1} & 1
\end{array}\right] .
$$

The linear system

The system can be converted to the triangular system

$$
\begin{array}{rlrlll}
x_{1}+x_{2} & & +3 x_{4} & = & 4, \\
& -x_{2}-x_{3} & -5 x_{4} & = & -7, \\
& & 3 x_{3} & +13 x_{4} & = & 13, \\
& & -13 x_{4} & = & -13,
\end{array}
$$

The multipliers $m_{i j}$ and the upper triangular matrix produce the factorization

$$
A=\left[\begin{array}{cccc}
1 & 1 & 0 & 3 \\
2 & 1 & -2 & 1 \\
3 & -1 & -1 & 2 \\
-1 & 2 & 3 & -1
\end{array}\right]=\left[\begin{array}{cccc}
1 & 0 & 0 & 0 \\
2 & 1 & 0 & 0 \\
3 & 4 & 1 & 0 \\
-1 & -3 & 0 & 1
\end{array}\right]\left[\begin{array}{cccc}
1 & 1 & 0 & 3 \\
0 & -1 & -1 & -5 \\
0 & 0 & 3 & 13 \\
0 & 0 & 0 & -13
\end{array}\right]=L U
$$

A matrix $A$ is positive definite if its symmetric and if $x^{t} A x>0$ for every $n$-dimensional vector $x \neq 0$.

The matrix $A$ is positive definite if and only if $A$ can be factored in the form $L D L^{t}$, where $L$ is lower triangular with 1's on its diagonal and $D$ is a diagonal matrix with positive diagonal entries.

The matrix $A$ is positive definite if and only if $A$ can be factored in the form $L L^{t}$, where $L$ is lower triangular with nonzero diagonal entries.

They offer computational advantages because only half the storage is needed and, in most cases, only half of the computation time is required for their solution.

## The matrix

$$
A=\left[\begin{array}{rll}
4 & -1 & 1 \\
-1 & 4.25 & 2.75 \\
1 & 2.75 & 3.5
\end{array}\right]
$$

is positive definite. The factorization $L D L^{t}$ of $A$ given in Algorithm 6.5 is

$$
A=L D L^{\prime}=\left[\begin{array}{cll}
1 & 0 & 0 \\
-0.25 & 1 & 0 \\
0.25 & 0.75 & 1
\end{array}\right]\left[\begin{array}{lll}
4 & 0 & 0 \\
0 & 4 & 0 \\
0 & 0 & 1
\end{array}\right]\left[\begin{array}{lll}
1 & -0.25 & 0.25 \\
0 & 1 & 0.75 \\
0 & 0 & 1
\end{array}\right]
$$

and Choleski's Algorithm 6.6 produces the factorization

$$
A=L L^{\prime}=\left[\begin{array}{cll}
2 & 0 & 0 \\
-0.5 & 2 & 0 \\
0.5 & 1.5 & 1
\end{array}\right]\left[\begin{array}{ccc}
2 & -0.5 & 0.5 \\
0 & 2 & 1.5 \\
0 & 0 & 1
\end{array}\right]
$$

### 1.4 Iterative techniques in Matrix Algebra

### 1.4.1 Gauss-Seidel

Suppose that for conciseness we limit ourselves to a $3 \times 3$ set of equations. The equations to solve yield $(A x=b)$ :

$$
\begin{align*}
& x_{1}=\frac{b_{1}-a_{12} x_{2}-a_{13} x_{3}}{a_{11}}  \tag{1.25}\\
& x_{2}=\frac{b_{2}-a_{21} x_{1}-a_{23} x_{3}}{a_{22}}  \tag{1.26}\\
& x_{3}=\frac{b_{3}-a_{31} x_{1}-a_{32} x_{2}}{a_{33}} \tag{1.27}
\end{align*}
$$

Now, we can start the solution process by choosing guesses for the $x$ 's. A simple way to obtain initial guesses is to assume that they are all zero. These zeros can be substituted into Eqs. which can be used to calculate a new value for $x_{1}=b_{1} / a_{11}$. Example:

$$
\begin{array}{rlrlr}
3 x_{1} & -0.1 x_{2} & -0.2 x_{3} & = & 7.85 \\
0.1 x_{1} & +7 x_{2} & -0.3 x_{3} & = & -19.3 \\
0.3 x_{1} & -0.2 x_{2} & +10 x_{3} & = & 71.4
\end{array}
$$

## 1. LINEAR SYSTEMS

Solve each of the equations for its unknown on the diagonal

$$
\begin{align*}
& x_{1}=\frac{7.85+0.1 x_{2}+0.2 x_{3}}{3}  \tag{1.28}\\
& x_{2}=\frac{-19.3-0.1 x_{1}+0.3 x_{3}}{7}  \tag{1.29}\\
& x_{3}=\frac{71.4-0.3 x_{1}+0.2 x_{2}}{10} \tag{1.30}
\end{align*}
$$

By assuming that $x_{2}$ and $x_{3}$ are zero, the first Eq. can be used to compute

$$
x_{1}=\frac{7.85+0+0}{3}=2.616667
$$

This value, along with the assumed value of $x_{3}=0$, can be substituted into the second to calculate

$$
x_{2}=\frac{-19.3-0.1(2.616667)+0}{7}=-2.794524
$$

and then use both of them to compute $x_{3}$ and so on. The true solution is $x_{1}=3, x_{2}=$ $-2.5, x_{3}=7$.


The diagonal coefficient in each of the equations must be larger that the sum of the absolute values of the other coefficients in the equation.
(hw: Tarea)
${ }^{* *}$ Find $\alpha$ 's such that has no solution, infinite number of solutions, the solution.

$$
\begin{align*}
x_{1}-x_{2}+\alpha x_{3} & =-2  \tag{1.31}\\
-x_{1}+2 x_{2}-\alpha x_{3} & =3  \tag{1.32}\\
\alpha x_{1}+x_{2}+x_{3} & =2 \tag{1.33}
\end{align*}
$$

Prove:

- The product of two symmetric matrices is symmetric
- The product of two $n \times n$ lower (upper) triangular matrix is lower (upper) triangular.
***Find all values of $\alpha$ that make the matrix singular

$$
A=\left[\begin{array}{ccc}
1 & -1 & \alpha \\
2 & 2 & 1 \\
0 & \alpha & -3 / 2
\end{array}\right]
$$

**Find $\alpha$ so that is positive definite

$$
A=\left[\begin{array}{ccc}
2 & \alpha & -1 \\
\alpha & 2 & 1 \\
-1 & 1 & 4
\end{array}\right]
$$

**Find all values of $\alpha$ and $\beta$ s.t. is singular, strictly diagonally dominant, symmetric, positive definite.

$$
A=\left[\begin{array}{lll}
\alpha & 1 & 0 \\
\beta & 2 & 1 \\
0 & 1 & 2
\end{array}\right]
$$

a) Factor the following matrix into LU decomposition
$\left[\begin{array}{rrrr}2.1756 & 4.0231 & -2.1732 & 5.1967 \\ -4.0231 & 6.0000 & 0 & 1.1973 \\ -1.0000 & -5.2107 & 1.1111 & 0 \\ 6.0235 & 7.0000 & 0 & -4.1561\end{array}\right]$

