## ME 310 <br> Numerical Methods

# Solving Systems of Linear Algebraic Equations 

These presentations are prepared by<br>Dr. Cuneyt Sert<br>Mechanical Engineering Department<br>Middle East Technical University<br>Ankara, Turkey<br>csert@metu.edu.tr

They can not be used without the permission of the author

## Math Introduction

\(\left.\begin{array}{l}\begin{array}{l}f_{1}\left(x_{1}, x_{2}, ···, x_{n}\right)=0 <br>
f_{2}\left(x_{1}, x_{2}, ···, x_{n}\right)=0 <br>
··· <br>

f_{n}\left(x_{1}, x_{2}, ···, x_{n}\right)=0\end{array}\end{array}\right\}\)| A general set of equations. |
| :--- |
| $n$ equations, $n$ unknowns. |

Linear Algebraic Equation: An equation of the form $f(x)=0$ where $f$ is a polynomial with linear terms.

$$
\left.\begin{array}{|c}
a_{11} x_{1}+a_{12} x_{2}+\ldots+a_{1 n} x_{n}=b_{1} \\
a_{21} x_{1}+a_{22} x_{2}+\ldots+a_{2 n} x_{n}=b_{2} \\
\ldots \\
a_{n 1} x_{1}+a_{n 2} x_{2}+\ldots+a_{n n} x_{n}=b_{n}
\end{array}\right\} \text { A general set of linear algebraic equations. }
$$

Matrix Form: $[\mathrm{A}]\{\mathrm{x}\}=\{\mathrm{b}\}$
[A] nxn Coefficient matrix
\{x\} nx1 Unknown vector
\{b\} nx1 Right-Hand-Side (RHS) vector

## Review of Matrices

$[A]=\left[\begin{array}{cccc}a_{11} & a_{12} & \cdots & a_{1 m} \\ a_{21} & a_{22} & \cdots & a_{2 m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n 1} & a_{n 2} & \cdots & a_{n m}\end{array}\right]_{n \times m} \longleftarrow 2^{\text {nd }}$ row $\quad$ Elements are indicated by $a_{i j}{ }^{i j}$

Square matrix: $[A]_{n \times m}$ is a square matrix if $n=m$. A system of $n$ equations with $n$ unknonws has a square coefficient matrix.

Main (principle) diagonal: of $[A]_{\mathrm{nxn}}$ consists of elements $\mathrm{a}_{\mathrm{i}} ; \mathrm{i}=1, \ldots, \mathrm{n}$
Symmetric matrix: If $\mathrm{a}_{\mathrm{ij}}=\mathrm{a}_{\mathbf{j i}} \rightarrow[\mathrm{A}]_{\mathrm{nxn}}$ is a symmetric matrix
Diagonal matrix: $[A]_{\mathrm{n} \times \mathrm{n}}$ is diagonal if $\mathrm{a}_{\mathrm{ij}}=0$ for all $\mathrm{i}=1, \ldots, \mathrm{n}$; $\mathrm{j}=1, \ldots, \mathrm{n}$ and $\mathrm{i} \neq \mathrm{j}$
Identity matrix: $[\mathrm{A}]_{\mathrm{nxn}}$ is an identity matrix if it is diagonal with $\mathrm{a}_{\mathrm{ii}}=1 \quad \mathrm{i}=1, \ldots, \mathrm{n}$. Shown as $[\mathrm{I}]$

## Review of Matrices (cont'd)

Upper triangular matrix: $[A]_{\mathrm{nxn}}$ is upper triangular if $\mathrm{a}_{\mathrm{ij}}=0 \mathrm{i}=1, \ldots, \mathrm{n} ; \mathrm{j}=1, \ldots, \mathrm{n}$ and $\mathrm{i}>\mathrm{j}$
Lower triangular matrix: $[A]_{\mathrm{nxn}}$ is lower triangular if $\mathrm{a}_{\mathrm{ij}}=0 \quad \mathrm{i}=1, \ldots, \mathrm{n} ; \mathrm{j}=1, \ldots, \mathrm{n}$ and $\mathrm{i}<\mathrm{j}$
Banded matrix: $[A]_{n \times n}$ is a banded matrix if $a_{i j}=0$ for all $j-i>H B W$ or $i-j>H B W$, where HBW is the half bandwidth.

Tridiagonal matrix: is a banded matrix with $\mathrm{HBW}=1$.
Inverse of a matrix: $[A]^{-1}$ is the inverse of $[A]_{n \times n}$ if $[A]^{-1}[A]=[I]$
Transpose of a matrix: $[B]$ is the transpose of $[A]_{n \times n}$ if $b_{i j}=a_{j i} \quad$ Shown as $[A]^{\prime}$ or $[A]^{\top}$
$\begin{array}{ll}\text { Matrix multiplication: } \quad[C]_{p \times s}=[A]_{p x r}[B]_{r \times s} \quad \rightarrow \quad \mathbf{c}_{\mathrm{ij}}=\sum_{\mathrm{k}=1}^{\mathrm{r}} \mathbf{a}_{\mathbf{i k}} \mathbf{b}_{\mathrm{kj}} \quad \mathrm{i}=1, \ldots, \mathrm{p} ; \mathrm{j}=1, \ldots, \mathrm{~s} \\ & \text { Note: }[\mathrm{A}][B] \neq[B][A]\end{array}$
Augmented matrix: is a special way of showing two matrices together.
For example $A=\left[\begin{array}{ll}a_{11} & a_{12} \\ a_{21} & a_{22}\end{array}\right]$ augmented with the column vector $B=\left[\begin{array}{l}b_{1} \\ b_{2}\end{array}\right]$ is $\left[\begin{array}{ll:l}a_{11} & a_{12} & b_{1} \\ a_{21} & a_{22} & b_{2}\end{array}\right]$
Determinant of a matrix: is a single number. Determinant of $[A]$ is shown as $|A|$.

## Graphical Method for Solving a Small ( $n \leq 3$ ) Set of Equations

- Consider a set of 2 equations

$$
\begin{aligned}
& a_{11} x_{1}+a_{12} x_{2}=b_{1} \\
& a_{21} x_{1}+a_{22} x_{2}=b_{2}
\end{aligned}
$$

- Plot these on the Cartesian coordinate system with axes $\mathrm{x}_{\mathbf{1}}$ and $\mathrm{x}_{\mathbf{2}}$.

$$
\begin{aligned}
& x_{2}=-\frac{a_{11}}{a_{12}} x_{1}+\frac{b_{1}}{a_{12}} \\
& x_{2}=-\frac{a_{21}}{a_{22}} x_{1}+\frac{b_{2}}{a_{22}}
\end{aligned}
$$

- For $n=3$, each equation will be a plane on a 3D coordinate system. Solution is the point where these planes intersect.
- For $n>3$, graphical solution is not practical.


## Graphical Method (cont'd)

Graphical Method is useful to illustrate:
(1) no solution

(2) infinitely many solutions

(3) ill-conditioned system


- In system (1) and (2), equations are linearly dependent.
- In system (3), the slopes of the lines are very close to each other.


## Mathematically

- Coefficient matrices of (1) \& (2) are singular. Their determinants are zero and their inverse do not exist.
- Coefficient matrix of (3) is almost singular. Its inverse is difficult to take. This system has a unique solution, which is not easy to determine numerically because of its extreme sensitivity to round-off errors.


## Cramer's Rule for Solving a Set of Equations

## Determinant of a system

- Determinant of a $2 \times 2$ matrix is $D=\left|\begin{array}{ll}a_{11} & \mathbf{a}_{12} \\ \mathbf{a}_{21} & \mathbf{a}_{22}\end{array}\right|=\mathbf{a}_{11} \mathbf{a}_{22}-\mathbf{a}_{12} \mathbf{a}_{21}$
- Determinant of a 3x3 matrix is $D=\mathbf{a}_{11}\left|\begin{array}{ll}\mathbf{a}_{22} & \mathbf{a}_{23} \\ \mathbf{a}_{32} & \mathbf{a}_{33}\end{array}\right|-\mathbf{a}_{12}\left|\begin{array}{ll}\mathbf{a}_{21} & \mathbf{a}_{23} \\ \mathbf{a}_{31} & \mathbf{a}_{33}\end{array}\right|+\mathbf{a}_{13}\left|\begin{array}{ll}\mathbf{a}_{21} & \mathbf{a}_{22} \\ \mathbf{a}_{31} & \mathbf{a}_{32}\end{array}\right|$
- Determinant of a general nxn matrix can be calculated recursively using the above pattern.
- Determinant of a singular system is zero. $\begin{aligned} \mathbf{x}_{1}-3 x_{2} & =5 \\ 2 x_{1}-6 x_{2} & =7\end{aligned}$
- Determinant of an illl-conditioned system is close to zero.

$$
2 x_{1}-3 x_{2}=5
$$

$$
3.98 x_{1}-6 x_{2}=7
$$

Warning: Multiply both equations of the above system with $100 \begin{aligned} & 200 x_{1}-300 x_{2}=500 \\ & 398 x_{1}-600 x_{2}=700\end{aligned}$
This system is as ill-conditioned as the previous one but it has a determinant 10000 times larger. Therefore we need to scale a system when we talk about the magnitude of its determinant. Details will come later.

## Cramer's Rule for Solving a Set of Equations (Contd)

Cramer's Rule: Each unknown is calculated as a fraction of two determinants. The denominator is the determinant of the system, D. The numerator is the determinant of a modified system obtained by replacing the column of coefficients of the unknown being calculated by the RHS vector.

For a $3 \times 3$ system

$$
x_{1}=\frac{\left|\begin{array}{lll}
b_{1} & a_{12} & a_{13} \\
b_{2} & a_{22} & a_{23} \\
b_{3} & a_{32} & a_{33}
\end{array}\right|}{D}
$$

$$
\mathbf{x}_{2}=\frac{\left|\begin{array}{lll}
\mathbf{a}_{11} & \mathbf{b}_{1} & a_{13} \\
\mathbf{a}_{21} & \mathbf{b}_{2} & a_{23} \\
\mathbf{a}_{31} & \mathbf{b}_{3} & a_{33}
\end{array}\right|}{\mathbf{D}}
$$

$$
\mathbf{x}_{3}=\frac{\left|\begin{array}{lll}
a_{11} & a_{12} & b_{1} \\
a_{21} & a_{22} & b_{2} \\
a_{31} & a_{32} & b_{3}
\end{array}\right|}{\mathbf{D}}
$$

- For a singular system $D=0 \rightarrow$ Solution can not be obtained.
- For large systems Cramer's rule is not practical because calculating determinants is costly.
- To solve an nxn system of equations, Cramer's rule needs $\mathrm{n}+1$ determinant evaluations. Using a recursive algorithm, determinant of an nun matrix requires $2 n!+2 n-1$ arithmetic operations ( $+,-, x, \dot{-}$ ). Therefore solving an nun system with the Cramer's Rule needs more than $(n+1)(2 n!+2 n-1)$. For a $20 \times 20$ system this means about $1 \times 10^{20}$ operations (Check these numbers).


## C and Matrices:

- A matrix is nothing but an array of arrays.
- In C array indices start from 0.
- C does not do check array bounds. Compilers might have switches for this.
- A 2D array (a matrix) is declared as double A[4][5] and its elements are reached as A[i][j]
- If you do not know the size of the matrices before starting the program, you need to use dynamic memory allocation with pointers. This can be quite confusing.


## Exercise 11:

(i) Write two functions to add and multiply two matrices. These functions should take two matrices and their sizes as input arguments and calculate a third matrix. They should check if the input matrices are suitable for addition or muliplication.
(ii) Write a main program. Generate two small matrices. Add and multiply them by calling proper functions.

## Exercise 12:

(i) Write a function that calculates the determinant of a matrix. Call this function recursively to solve systems of equations using the Cramer's Rule.
(ii) Use this program to solve a $10 \times 10$ set of equations. Generate the coefficient matrix of the system inside a loop. Make sure that your system is not singular. How long it takes to solve this system? Try solving larger systems.

## Elimination of Unknowns Method

Example 11: Given a $2 \times 2$ set of equations:

$$
\begin{aligned}
& 2.5 x_{1}+6.2 x_{2}=3.0 \\
& 4.8 x_{1}-8.6 x_{2}=5.5
\end{aligned}
$$

- Multiply the $1^{\text {st }}$ eqn by 8.6 and the $2^{\text {nd }}$ eqn by 6.2 :

$$
\begin{aligned}
& 21.50 x_{1}+53.32 x_{2}=25.8 \\
& 29.76 x_{1}-53.32 x_{2}=34.1
\end{aligned}
$$

- Add these equations: $51.26 \mathrm{x}_{1}+0 \mathrm{x}_{2}=59.9$
- Solve for $\mathrm{x}_{\mathbf{1}}$ : $\mathbf{x}_{1}=59.9 / 51.26=1.168552478$
$\bullet$ Using the $1^{\text {st }}$ eqn solve for $\mathrm{x}_{2}: \quad \mathbf{x}_{2}=(3.0-2.5 * 1.168552478) / 6.2=0.01268045242$
- Check if these satisfy the $2^{\text {nd }}$ eqn: $4.8 * 1.168552478-8.6 * 0.01268045242=5.500000004$
(Difference is due to the round-off errors).


## Naive Gauss Elimination Method

- It is a formalized way of the previous elimination technique.
- Consider the following system of $n$ equations.

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

Step 0 (optional): Form the augmented matrix of [A|B].

Step 1 Forward Elimination: Reduce the system to an upper triangular system.
(1.1) First eliminate $\mathrm{x}_{1}$ from $2^{\text {nd }}$ to $\mathrm{n}^{\text {th }}$ equations.

- Multiply the $1^{\text {st }}$ eqn. by $a_{21} / a_{11}$ \& subtract it from the $2^{\text {nd }}$ equation. This is the new $2^{\text {nd }}$ eqn.
- Multiply the $1^{\text {st }}$ eqn. by $\mathrm{a}_{\mathbf{3 1}} / a_{1 \mathbf{1 1}}$ \& subtract it from the $3^{\text {rd }}$ equation. This is the new $3^{\text {rd }}$ eqn.
- Multiply the $1^{\text {st }}$ eqn. by $a_{n \mathbf{1}} / a_{\mathbf{1 1}}$ \& subtract it from the $n^{\text {th }}$ equation. This is the new $n^{\text {th }}$ eqn.

Important: In these steps the $1^{\text {st }}$ eqn is the pivot equation and $\mathrm{a}_{\mathbf{1 1}}$ is the pivot element. Note that a division by zero may occur if the pivot element is zero. Naive-Gauss Elimination does not check for this.

## Naive Gauss Elimination Method (cont'd)

The modified system is $\left[\begin{array}{ccccc}a_{11} & a_{12} & a_{13} & \cdots & a_{1 n} \\ 0 & a_{22}^{\prime} & a_{23}^{\prime} & \cdots & a_{2 n}^{\prime} \\ 0 & a_{32}^{\prime} & a_{33}^{\prime} & \cdots & a_{3 n}^{\prime} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n 2}^{\prime} & a_{n 3}^{\prime} & \cdots & a_{n n}^{\prime}\end{array}\right]\left\{\begin{array}{c}x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n}\end{array}\right\}=\left\{\begin{array}{c}b_{1} \\ b_{2}^{\prime} \\ b_{3}^{\prime} \\ \vdots \\ b_{n}^{\prime}\end{array}\right\}$
' indicates that the system is modified once.
(1.2) Now eliminate $x_{2}$ from $3^{\text {rd }}$ to $n^{\text {th }}$ equations.

The modified system is $\left[\begin{array}{ccccc}a_{11} & a_{12} & a_{13} & \cdots & a_{1 n} \\ 0 & a_{22}^{\prime} & a_{23}^{\prime} & \cdots & a_{2 n}^{\prime} \\ 0 & 0 & a_{33}^{\prime \prime} & \cdots & a_{3 n}^{\prime \prime} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n 3}^{\prime \prime} & \cdots & a_{n n}^{\prime \prime}\end{array}\right]\left\{\begin{array}{c}x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n}\end{array}\right\}=\left\{\begin{array}{c}b_{1} \\ b_{2}^{\prime} \\ b_{3}^{\prime \prime} \\ \vdots \\ b_{n}^{\prime \prime}\end{array}\right\}$
" indicates that the system is modified once.

Repeat (1.1) and (1.2) upto (1.n-1).

At the end of Step 1, we will get this upper triangular system

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \cdots & a_{1 n} \\
0 & a_{22} & a_{23} & \cdots & a_{2 n} \\
0 & 0 & a_{33} & \cdots & a_{3 n} \\
0 & 0 & 0 & \ddots & \vdots \\
0 & 0 & 0 & 0 & a_{n n}
\end{array}\right]\{x\}=\{b\}
$$

Primes are removed for clarity.

## Naive Gauss Elimination Method (cont'd)

Step 2 Back substitution: Find the unknowns starting from the last equation.
(2.1) Last equation involves only $x_{n}$. Solve for it.
(2.1) Use this $\mathrm{X}_{\mathrm{n}}$ in the $(\mathrm{n}-1)^{\text {th }}$ equation and solve for $\mathrm{X}_{\mathrm{n}-1}$.
(2.n) Use all previously calculated $x$ values in the $1^{\text {st }}$ eqn and solve for $x_{1}$.

Example 12: Solve the following system using Naive Gauss Elimination.

$$
\begin{aligned}
6 x_{1}-2 x_{2}+2 x_{3}+4 x_{4}= & 16 \\
12 x_{1}-8 x_{2}+6 x_{3}+10 x_{4}= & 26 \\
3 x_{1}-13 x_{2}+9 x_{3}+3 x_{4}= & -19 \\
-6 x_{1}+4 x_{2}+x_{3}-18 x_{4}= & -34
\end{aligned}
$$

Step 0: Form the augmented matrix

| 6 | -2 | 2 | 4 | 16 |
| ---: | ---: | ---: | ---: | ---: |
| 12 | -8 | 6 | 10 | 26 |
| 3 | -13 | 9 | 3 | -19 |
| -6 | 4 | 1 | -18 | -34 |

## Naive Gauss Elimination Method (cont'd)

Step 1: Forward elimination
(1.1) Eliminate $\mathrm{X}_{1}$

| 6 | -2 | 2 | 4 | 16 |
| ---: | ---: | ---: | ---: | ---: |
| 0 | -4 | 2 | 2 | 1 |
| 0 | -12 | 8 | 1 | 1 |
| 0 | 2 | 3 | -14 | 1 |
| 0 | -18 |  |  |  |

(Does not change. Pivot is 6)
(1.2) Eliminate $x_{2}$

$$
\begin{array}{rrrr|r}
6 & -2 & 2 & 4 & 16 \\
0 & -4 & 2 & 2 & 1 \\
0 & 0 & 2 & -5 & -9 \\
0 & 0 & 4 & -13 & -21
\end{array}
$$

(Does not change.)
(Does not change. Pivot is -4)
(1.3) Eliminate $x_{3}$

$$
\begin{array}{rrrr|r}
6 & -2 & 2 & 4 & 16 \\
0 & -4 & 2 & 2 & 1 \\
0 & 0 & 2 & -5 & -9 \\
0 & 0 & 0 & -3 & -3
\end{array}
$$

(Does not change.)
(Does not change.)
(Does not change. Pivot is 2)

Step 2: Back substitution
(2.1) Find $x_{4}$

$$
x_{4}=(-3) /(-3)
$$

$$
=1
$$

(2.2) Find $x_{3}$
(2.3) Find $x_{2}$
$x_{2}=(-6-2 *(-2)-2 * 1) /(-4)=1$
(2.4) Find $x_{1} \quad x_{1}=(16+2 * 1-2 *(-2)-4 * 1) / 6=3$

## Pseudocode for the Naive Gauss Elimination Method

For a general nxn system $[A]\{x\}=\{B\}$

## Forward Elimination

LOOP $k$ from 1 to $n-1$
LOOP i from $k+1$ to $n$
FACTOR $=\mathrm{A}_{\mathbf{i k}} / \mathrm{A}_{\mathbf{k k}}$
LOOP j from $\mathrm{k}+1$ to n

$$
A_{i j}=A_{i j}-\text { FACTOR }^{*} A_{\mathbf{k j}}
$$

END LOOP

$$
\mathrm{B}_{\mathbf{i}}=\mathrm{B}_{\mathbf{i}}-\text { FACTOR } * \mathrm{~B}_{\mathbf{k}}
$$

ENDLOOP

Back Substitution
$X_{n}=B_{n} / A_{n}$
LOOP i from $n-1$ to 1
SUM $=0.0$
LOOP j from $\mathrm{i}+1$ to n SUM $=\operatorname{SUM}+\mathrm{A}_{\mathrm{ij}} * X_{\mathrm{j}}$
END LOOP
$X_{i}=\left(B_{i}-S U M\right) / A_{i i}$
ENDLOOP

## ENDLOOP

Exercise 13: Implement this in C. Write a main program and two functions. You need to know how to pass matrices to the functions.

## Operation Count for the Naive Gauss Elimination Method

Let's count the FLOPS (floating point operations). Consider only multiplications and divisions, since they are more expensive to perform.


Example 13:

| n | $* \& /$ in FE | $* \& /$ in BS | Total $* \& /$ | $\mathrm{n}^{3} / 3$ | $\%$ due to FE |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 10 | 375 | 55 | 430 | 333 | $87.2 \%$ |
| 100 | 338250 | 5050 | 343300 | 333333 | $98.5 \%$ |
| 1000 | 3.34 E 8 | 500500 | 3.34 E 8 | 3.33 E 8 | $99.8 \%$ |

## Pivoting

- In Naive Gauss Elimination, a division by zero occurs if the pivot element is zero. Note that zero pivot elements may be created during the elimination step even if they are not present in the original matrix.
- Pivoting is used to avoid this problem. We interchange rows and columns at each step to put the coefficient with the largest magnitude on the diagonal.
- In addition to avoiding the division by zero problem, pivoting reduces the round-off errors. It makes the solution of ill-conditioned systems easier.
- Complete pivoting uses both row and column interchanges. It is not used frequently.
- Partial pivoting uses only row interchanges. We will use this.
- When there are large differences in magnitude of coefficients in one equation compared to the other equations we may also need scaling. Details will come later.


## Pivoting Example

Example 14: Solve the following system using Gauss Elimination with pivoting.

$$
\begin{aligned}
2 x_{2}+3 x_{4}= & 0 \\
2 \mathbf{x}_{1}+2 x_{2}+3 x_{3}+2 x_{4}= & -2 \\
4 \mathbf{x}_{1}-3 x_{2}+\mathbf{x}_{4}= & -7 \\
6 \mathbf{x}_{1}+\mathbf{x}_{2}-6 \mathbf{x}_{3}-5 \mathbf{x}_{4}= & 6
\end{aligned}
$$

Step 0: Form the augmented matrix

| 0 | 2 | 0 | 1 | 1 | 0 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 2 | 2 | 3 | 2 | 1 | -2 |
| 4 | -3 | 0 | 1 | 1 | -7 |
| 6 | 1 | -6 | -5 | 1 | 6 |

Step 1: Forward Elimination
(1.1) Eliminate $x_{1}$. But the pivot element is 0 . We have to interchange the $1^{\text {st }}$ row with one of the rows below it. Interchange it with the $4^{\text {th }}$ row because 6 is the largest possible pivot.

| 6 | 1 | -6 | -5 | 1 | 6 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 2 | 2 | 3 | 2 | 1 | -2 |
| 4 | -3 | 0 | 1 | 1 | -7 |
| 0 | 2 | 0 | 1 | 1 | 0 |


| 6 | 1 | -6 | -5 | $\mid$ |
| :---: | :---: | ---: | :--- | ---: |
| 0 | 1.6667 | 5 | 3.6667 | 1 |
| 0 | -3.6667 | 4 | 4.3333 | 1 |
| 0 | 2 | 0 | 1 | 11 |
| 0 | 0 |  |  |  |

## Pivoting Example (cont'd)

(1.2) Eliminate $x_{2}$.from the $3^{\text {rd }}$ and $4^{\text {th }}$ eqns. Pivot element is 1.6667 . There is no division by zero problem. Still we will perform pivoting to reduce round-off errors. Interchange the $2^{\text {nd }}$ and $3^{\text {rd }}$ rows. Note that complete pivoting would interchange $2^{\text {nd }}$ and $3^{\text {rd }}$ columns.

| 6 | 1 | -6 | -5 | 16 | Eliminate $\mathrm{x}_{2}$ | 6 | 1 | -6 | -5 |  | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | -3.6667 | 4 | 4.3333 | \| -11 |  | 0 | -3.6667 | 4 | 4.3333 | I | -11 |
| 0 | 1.6667 | 5 | 3.6667 | \| -4 |  | 0 | 0 | 6.8182 | 5.6364 | 1 | -9.0001 |
| 0 | 2 | 0 | 1 | 10 |  | 0 | 0 | 2.1818 | 3.3636 | I | -5.9999 |

(1.3) Eliminate $x_{3} .6 .8182>2.1818$, therefore no pivoting is necessary.

| 6 | 1 | -6 | -5 | 6 |
| :---: | :---: | :---: | :---: | :---: |
| 0 | -3.6667 | 4 | 4.3333 | -11 |
| 0 | 0 | 6.8182 | 5.6364 | -9.0001 |
| 0 | 0 | 0 | 1.5600 | -3.1199 |

Step 2: Back substitution
$\mathrm{x}_{4}=-3.1199 / 1.5600=\mathbf{- 1 . 9 9 9 9}$
$x_{3}=[-9.0001-5.6364 *(-1.9999)] / 6.8182=\mathbf{0 . 3 3 3 2 5}$
$x_{2}=[-11-4.3333 *(-1.9999)-4 * 0.33325] /-3.6667=1.0000$
$\mathrm{x}_{\mathbf{1}}=\left[6-(-5) *(-1.9999)-(-6) * 0.33325-1^{*} 1.0000\right] / 6=\mathbf{- 0 . 5 0 0 0 0}$
Exact solution is $x=\left[\begin{array}{llll}-2 & 1 / 3 & 1 & -0.5\end{array}\right]^{\top} \quad$. Use more than 5 sig. figs. to reduce round-off errors.

## Scaling

- Normalize the equations so that the maximum coefficient in every row is equal to 1.0. That is, divide each row by the coefficient in that row with the maximum magnitude.
- It is advised to scale a system before calculating its determinant. This is especially important if we are calculating the determinant to see if the system is ill-conditioned or not.
- Consider the following systems

$$
\begin{array}{rr}
2 \mathbf{x}_{1}-3 \mathbf{x}_{2}=5 & 20 \mathbf{x}_{1}-30 \mathbf{x}_{2}=50 \\
3.98 \mathbf{x}_{1}-6 \mathbf{x}_{2}=7 & 39.8 \mathbf{x}_{1}-60 \mathbf{x}_{2}=70
\end{array}
$$

- They are actually the same system. In the second one the equations are multiplied by 10.
- Determinant of the $1^{\text {st }}$ system is $2(-6)-(-3)(3.98)=-0.06$, which is close to zero.
- Determinant of the $2^{\text {nd }}$ system is $20(-60)-(-30)(39.8)=-6$, which is not that close to zero.
- So is this system ill-conditioned or not?
- Scale this system. They are the same, use the $1^{\text {st }}$ one.

$$
\begin{array}{r}
0.6667 \mathbf{x}_{1}+\mathbf{x}_{2}=-1.6667 \\
-0.6633 \mathbf{x}_{1}+\mathbf{x}_{2}=-1.1667
\end{array}
$$

- Now calculate the determinant as $0.6667^{*} 1-1^{*}(-0.6633)=1.33$. Use this value in judging the systems condition. Note that "How close to zero?" is still an open question. There are other ways to determine a systems condition (See page 277).


## Scaled Partial Pivoting

- Scaling is also useful when some rows have coefficients that are large compared to those in other rows.
- Consider the following system

$$
\begin{aligned}
2 \mathbf{x}_{1}+100000 \mathbf{x}_{2} & =100000 \\
\mathbf{x}_{1}+\quad \mathbf{x}_{2} & =2
\end{aligned}
$$

$$
\text { Exact solution is }(1.00002,0.99998)
$$

(a) If we solve this system with Gauss Elimination, no pivoting is necessary (2 is larger than 1). Use only 3 sig. figs to emphasize the round-off errors.

$$
\begin{array}{rlrl}
2.00 * 10^{0} \mathbf{x}_{1} & +1.00 * 10^{5} \mathbf{x}_{2} & =1.00 * 10^{5} \\
-5.00 * 10^{4} \mathbf{x}_{2} & =-5.00 * 10^{4}
\end{array} \quad \longrightarrow \quad \begin{aligned}
& \mathbf{x}_{1}=0.00 * 10^{1} \\
& \mathbf{x}_{2}=1.00 * 10^{1}
\end{aligned} \quad \text { WRONG }
$$

(b) First scale the system and than solve with Gauss Elimination.

$$
\begin{aligned}
2.00 * 10^{-5} \mathbf{x}_{1}+\mathbf{x}_{2} & =1 \\
\mathbf{x}_{1}+\mathbf{x}_{2} & =2
\end{aligned}
$$

This system now needs pivoting. Interchange the rows and solve.

$$
\begin{aligned}
2.00 * 10^{-5} \mathbf{x}_{1}+\mathbf{x}_{2}=1.00 * 10^{0} \\
\mathbf{x}_{1}+\mathbf{x}_{2}=2.00 * 10^{0}
\end{aligned} \quad \longrightarrow \quad \begin{aligned}
\mathbf{x}_{1}+\mathbf{x}_{2} & =2 \\
\mathbf{x}_{2} & =1
\end{aligned} \quad \longrightarrow \quad \begin{aligned}
& \mathbf{x} 1
\end{aligned}=1.00 \quad \text { OK }
$$

Conclusion: Scaling showed that pivoting is necessary. But scaling itself is not necessary (pivot the original system and solve). Scaling also introduces additional round-off errors. Therefore use scaling to decide whether pivoting is necessary or not but than use the original coefficients.

## Example for Gauss Elimination with Scaled Partial Pivoting

Example 15: Solve the following system using Gauss Elimination with scaled partial pivoting. Keep numbers as fractions of integers to eliminate round-off errors.

| 3 | -13 | 9 | 3 | 1 | -19 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| -6 | 4 | 1 | -18 | 1 | -34 |
| 6 | -2 | 2 | 4 | 1 | 16 |
| 12 | -8 | 6 | 10 | 1 | 26 |

Start by forming the scale vector. It has the largest coefficient (in magnitude) of each row.

```
SV = {lllllll
```

This scale vector will be updated if we interchange rows during pivoting.

Step 1: Forward Elimination

## Example for Gauss Elimination with Scaled Pivoting (cont'd)

(1.1) Compare scaled coefficients $3 / 13,6 / 18,6 / 6,12 / 12$. Third one is the largest (actually fourth one is the same but we use the first occurance). Interchange rows 1 and 3.

| 6 | -2 | 2 | 4 | 1 | 16 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| -6 | 4 | 1 | -18 | 1 | -34 |
| 3 | -13 | 9 | 3 | 1 | -19 |
| 12 | -8 | 6 | 10 | 1 | 26 |

Update the scale vector $\quad S V=\left\{\begin{array}{llll}6 & 18 & 13 & 12\end{array}\right\}$
Eliminate $\mathrm{x}_{1}$.
Subtract (-6/6) times row 1 from row 2.
Subtract (3/6) times row 1 from row 3.
Subtract (12/6) times row 1 from row 4.
Resulting system is

| 6 | -2 | 2 | 4 | 1 | 16 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 0 | 2 | 3 | -14 | 1 | -18 |
| 0 | -12 | 8 | 1 | 1 | -27 |
| 0 | -4 | 2 | 2 | 1 | -6 |

## Example for Gauss Elimination with Scaled Pivoting (cont'd)

(1.2) Compare scaled coefficients $2 / 18,12 / 13,4 / 12$. Second one is the largest. Interchange rows 2 and 3.

| 6 | -2 | 2 | 4 | 1 | 16 |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 0 | -12 | 8 | 1 | 1 | -27 |
| 0 | 2 | 3 | -14 | 1 | -18 |
| 0 | -4 | 2 | 2 | 1 | -6 |

Update the scale vector $\quad S V=\left\{\begin{array}{llll}6 & 13 & 18 & 12\end{array}\right\}$

Eliminate $\mathrm{x}_{2}$.
Subtract (2/(-12)) times row 2 from row 3.
Subtract ((-4)/(-12)) times row 2 from row 4.
Resulting system is

| 6 | -2 | 2 | 4 | 16 |  |
| ---: | ---: | :---: | :---: | :--- | :---: |
| 0 | -12 | 8 | 1 | 1 | -27 |
| 0 | 0 | $13 / 3$ | $-83 / 6$ | 1 | $-45 / 2$ |
| 0 | 0 | $-2 / 3$ | $5 / 3$ | 1 | 3 |

## Example for Gauss Elimination with Scaled Pivoting (cont'd)

(1.3) Compare scaled coefficients (13/3)/18, (2/3)/12. First one is larger. No need for pivoting.

Scale vector remains the same $\quad \mathrm{SV}=\left\{\begin{array}{llll}6 & 13 & 18 & 12\end{array}\right\}$

Eliminate $x_{3}$.
Subtract ((-2/3)/(13/3)) times row 3 from row 4.
Resulting system is

| 6 | -2 | 2 | 4 | 16 |  |
| :---: | ---: | :---: | :---: | :--- | :---: |
| 0 | -12 | 8 | 1 | 1 | -27 |
| 0 | 0 | $13 / 3$ | $-83 / 6$ | $\mid$ | $-45 / 2$ |
| 0 | 0 | 0 | $-6 / 13$ |  | $-6 / 13$ |

Step 2: Back substitution
Equation $4 \rightarrow x_{4}=1$
Equation $3 \rightarrow x_{3}=-2$
Equation $2 \rightarrow x_{2}=1$
Equation $1 \rightarrow x_{1}=3$
These are exact results because round-off errors are eliminated by not using floating point numbers ${ }_{25}$

## Ill-conditioned Systems

- They have almost singular coefficient matrices.
- They have a unique solution.
- Consider the following $3 \times 3$ system

| 3.02 | -1.05 | 2.53 | -1.61 |
| ---: | ---: | ---: | ---: |
| 4.33 | 0.56 | -1.87 | 7.23 |
| -0.83 | -0.54 | 1.47 | -3.38 |

The solution of this system is $\left[\begin{array}{lll}1 & 2 & -1\end{array}\right]^{\top}$

- Change $b_{1}$ from -1.61 to -1.60 . The solutions changes to $\left[\begin{array}{llll}1.0566 & 4.0051 & -0.2315\end{array}\right]^{\top}$
- Or change $\mathrm{a}_{11}$ from 3.02 to 3.00 . The solutions changes to $\left[\begin{array}{lll}1.1277 & 6.5221 & 0.7333\end{array}\right]^{\top}$
- This is a typical ill-conditioned system. Its solution is very sensitive to the changes in the coefficient matrix or the right-hand-side vector.
- This means it is very sensitive to round-off errors. Double precision must be used to reduce round-off errors as much as possible.
- Scaled pivoting should also be used to decrease round-off errors.
- Fortunately not many engineering problems will result in an ill-conditioned system.


## Other Uses of Gauss Elimination

- Gives the LU decomposition of A such that [L][U]=[A]. LU decomposition is useful if we are solving many systems with the same coefficient matrix A but different right-hand-side vectors (See page 266).
- It can be used to calculate the determinant of a matrix. At the end of the Forward Elimination step we get an upper triangular matrix. For this matrix the determinant is just the multiplication of diagonal elements. If we interchanged rows $m$ times, than the deteminant can be calculated as

$$
|A|=(-1)^{m} * a_{11} * a_{22} * \ldots a_{n n}
$$

Example 16: Remember the example we used to describe pivoting. The A matrix was

| 0 | 2 | 0 | 1 |
| ---: | ---: | ---: | ---: |
| 2 | 2 | 3 | 2 |
| 4 | -3 | 0 | 1 |
| 6 | 1 | -6 | -5 |

After the Forward Elimination step we found the following upper triangular matrix.

| 6 | 1 | -6 | -5 |
| :---: | :---: | :---: | :---: |
| 0 | -3.6667 | 4 | 4.3333 |
| 0 | 0 | 6.8182 | 5.6364 |
| 0 | 0 | 0 | 1.5600 |

To get this, we used pivoting and interchanged rows twice. Therefore the determinant of $A$ is $|A|=(-1)^{2} * 6 *(-3.6667) * 6.8182 * 1.56=-234.0028$

## Gauss-Jordan Method

- This is another elimination technique. It is a variation of Gauss Elimination.
- The difference is, when an unknown is eliminated, it is eliminated from all other equations, not just the subsequent ones. At the same time all rows are normalized by dividing them to their pivot element.
- At the end of the forward elimination step Gauss-Jordan method yields an identity matrix, not an upper triangular one.
- There is no need for back substitution. Right-hand-side vector has the results.

Example 17: Solve the following $4 \times 4$ system using G-J method with pivoting. Note that this is the same system that we used to demonstrate Gauss Elimination with pivoting.

| 0 | 2 | 0 | 1 | 1 |
| ---: | ---: | ---: | ---: | ---: |
| 2 | 2 | 3 | 2 | -2 |
| 4 | -3 | 0 | 1 | -7 |
| 6 | 1 | -6 | -5 | 6 |

- Interchange rows 1 and 4, divide the new first row by 6 and eliminate $\mathrm{x}_{1}$ from the $2^{\text {nd }}, 3^{\text {rd }}$ and $4^{\text {th }}$ equations.

| 1 | 0.1667 | -1 | -0.8333 | 1 |
| ---: | ---: | ---: | ---: | ---: |
| 0 | 1.6667 | 5 | 3.6667 | -4 |
| 0 | -3.6667 | 4 | 4.3333 | -11 |
| 0 | 2 | 0 | 1 | 1 |

## Gauss-Jordan Method (cont'd)

- Interchange rows 2 and 3, divide the new second row by -3.6667 and eliminate $x_{2}$ from the $1^{\text {st }}, 3^{\text {rd }}$ and $4^{\text {th }}$ equations.

| 1 | 0 | -0.8182 | -0.6364 | 0.5 |
| ---: | ---: | ---: | ---: | :---: |
| 0 | 1 | -1.0909 | -1.1818 | $\mid$ |
| 0 | 0 | 6.8182 | 5.6364 | -9 |
| 0 | 0 | 2.1818 | 3.3636 |  |
|  |  | -6 |  |  |

- No pivoting is required. Divide the third row by 6.8182 and eliminate $x_{3}$ from the $1^{\text {st }}, 2^{\text {nd }}$ and $4^{\text {th }}$ equations.

| 1 | 0 | 0 | 0.04 | 0.58 |  |
| :--- | :--- | :--- | :--- | :--- | ---: |
| 0 | 1 | 0 | -0.280 | 1 | 1.56 |
| 0 | 0 | 1 | 0 | 1 | -1.32 |
| 0 | 0 | 0 | 1.5599 | -3.12 |  |

- Divide the last row by 1.5599 and eliminate $x_{4}$ from the $1^{\text {st }}, 2^{\text {nd }}$ and $3^{\text {rd }}$ equations.

| 1 | 0 | 0 | 0 | $\mid$ | -0.5 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 0 | $\mid$ | 1.0001 |
| 0 | 0 | 1 | 0 | 1 | 0.3333 |
| 0 | 0 | 0 | 1 | 1 | -2 |

- Right-hand-side vector is the solution. No back substitution is required.
- Gauss-Jordan requires almost 50\% more operations than Gauss Elimination ( $n^{3} / 2$ instead of $n^{3} / 3$ ).


## Calculating the Inverse of a Matrix with Gauss-Jordan

- Calculating the inverse of a matrix is important if we want to solve many systems with the same coefficient matrix, but different right-hand-side vectors.
- To take the inverse of A, augment it with an identity matrix and apply the Gauss-Jordan method.

Example 18: Find the inverse of the following matrix.

$$
A=\begin{array}{rrr}
1 & -1 & 2 \\
3 & 0 & 1 \\
1 & 0 & 2
\end{array}
$$

- Augment A with a $3 \times 3$ identity matrix.

| 1 | -1 | 2 | 1 | 1 | 0 | 0 |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 3 | 0 | 1 | 1 | 0 | 1 | 0 |
| 1 | 0 | 2 | 1 | 0 | 0 | 1 |

- Apply the Gauss-Jordan method to this system to get

| 1 | 0 | 0 | $\mid$ | 0 | 0.4 | -0.2 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 1 | -1 | 0 | 1 |
| 0 | 0 | 1 | 1 | 0 | -0.2 | 0.6 |

- $3 \times 3$ matrix at the right is the inverse of A . This inverse can now be used to solve a system with the coefficient matrix $A$ and different right-hand-side vectors as $\{x\}=[A]^{-1}\{B\}$
- LU decomposition can be used for the same purpose and it is more efficient (See page 273).


## Iterative Methods - Gauss-Seidel Method

- Gauss Elimination and its variants are called direct methods. They are not preferred for large systems.
- Iterative methods start with an initial solution vector and iteratively converge to the true solution.
- They stop when the pre-specified tolerance is reached and round-off errors are not an issue.
- Given the system $[A]\{x\}=\{B\}$ and starting values $\{x\}^{0}$, Gauss-Seidel uses the first equation to solve for $\mathrm{X}_{1}$, second for $\mathrm{X}_{2}$, etc.

$$
\begin{aligned}
& x_{1}=\left(b_{1}-a_{12} x_{2}-a_{13} x_{3}-\ldots .-a_{1 n} x_{n}\right) / a_{11} \\
& x_{2}=\left(b_{2}-a_{21} x_{1}-a_{23} x_{3}-\ldots . a_{2 n} x_{n}\right) / a_{22}
\end{aligned}
$$

$$
x_{n}=\left(b_{n}-a_{n 1} x_{1}-a_{n 2} x_{2}-\ldots .-a_{(n-1)(n-1)} x_{n-1}\right) / a_{n n}
$$

After the first iteration you get $\{x\}^{1}$. Use these values to start a new iteration. Repeat until the tolerance is satisfied as

$$
\left|\varepsilon_{a, i}\right|=\left|\frac{x_{i}^{k}-x_{i}^{k-1}}{x_{i}^{k}}\right| 100 \%<\varepsilon_{s}
$$

for all the unknowns ( $\mathrm{i}=1, \ldots, \mathrm{n}$ ), where k and $\mathrm{k}-1$ represent the present and previous iterations.

## Gauss-Seidel Example

Solve the following system using the Gauss-Seidel Method

$$
\begin{array}{rr}
6 \mathbf{x}_{1}-2 \mathbf{x}_{2}+\mathbf{x}_{3}= & 11 \\
-2 \mathbf{x}_{1}+7 x_{2}+2 x_{3}= & 5 \\
\mathbf{x}_{1}+2 \mathbf{x}_{2}-5 x_{3}= & -1
\end{array}
$$

$$
-2 \mathbf{x}_{1}+7 \mathbf{x}_{2}+2 \mathbf{x}_{3}=5 \quad \text { starting with } x_{1}{ }^{0}=x_{2}{ }^{0}=x_{3}{ }^{0}=0.0
$$

- Rearrange the equations

$$
\begin{aligned}
& \mathbf{x}_{1}=\left(11+2 \mathbf{x}_{2}-\mathbf{x}_{3}\right) / 6 \\
& \mathbf{x}_{2}=\left(5+2 \mathbf{x}_{1}-2 \mathbf{x}_{3}\right) / 7 \\
& \mathbf{x}_{3}=\left(1+\mathbf{x}_{1}+2 \mathbf{x}_{2}\right) / 5
\end{aligned}
$$

- First iteration

$$
\begin{aligned}
& \mathbf{x}_{1}{ }^{1}=\left(11+2 \mathbf{x}_{2}{ }^{0}-\mathbf{x}_{3}{ }^{0}\right) / 6=(11+0-0) / 6=1.833 \\
& \mathbf{x}_{2}{ }^{1}=\left(5+2 \mathbf{x}_{1}{ }^{1}-2 \mathbf{x}_{3}{ }^{0}\right) / 7=(5+2 * 1.8333-0) / 7=1.238 \\
& \mathbf{x}_{3}{ }^{1}=\left(1+\mathbf{x}_{1}{ }^{1}+2 \mathbf{x}_{2}{ }^{1}\right) / 5=(1+1.8333+2 * 1.2381) / 5=1.062
\end{aligned}
$$

- Second iteration

$$
\begin{aligned}
& \mathbf{x}_{1}^{2}=\left(11+2 \mathbf{x}_{2}^{1}-\mathbf{x}_{3}^{1}\right) / 6=(11+2 * 1.238-1.062) / 6=2.069 \\
& \mathbf{x}_{2}^{2}=\left(5+2 \mathbf{x}_{1}^{2}-2 \mathbf{x}_{3}^{1}\right) / 7=(5+2 \star 2.069-2 \star 1.062) / 7=1.002 \\
& \mathbf{x}_{3}^{2}=\left(1+\mathbf{x}_{1}^{2}+2 \mathbf{x}_{2}^{2}\right) / 5=(1+2.069+2 * 1.002) / 5=1.015
\end{aligned}
$$

- Continue like this to get (Do not forget to check convergence using the specified tolerance)

|  | Zeroth | First | Second | Third | Fourth | Fifth |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{x}_{1}$ | 0.000 | 1.833 | 2.069 | 1.998 | 1.999 | 2.000 |
| $\mathrm{x}_{2}$ | 0.000 | 1.238 | 1.002 | 0.995 | 1.000 | 1.000 |
| $\mathrm{x}_{3}$ | 0.000 | 1.062 | 1.015 | 0.998 | 1.000 | 1.000 |

## Jacobi Method

- Gauss- Seidel always uses the newest available x values. Jacobi Method uses x values from the previous iteration.

Example 19: Repeat the previous example using the Jacobi method.

- Rearrange the equations

$$
\begin{aligned}
& \mathbf{x}_{1}=\left(11+2 \mathbf{x}_{2}-\mathbf{x}_{3}\right) / 6 \\
& \mathbf{x}_{2}=\left(5+2 \mathbf{x}_{1}-2 \mathbf{x}_{3}\right) / 7 \\
& \mathbf{x}_{3}=\left(1+\mathbf{x}_{1}+2 \mathbf{x}_{2}\right) / 5
\end{aligned}
$$

- First iteration (use $x^{0}$ values)

$$
\begin{aligned}
& \mathbf{x}_{1}^{1}=\left(11+2 \mathbf{x}_{2}{ }^{0}-\mathbf{x}_{3}^{0}\right) / 6=(11+0-0) / 6=1.833 \\
& \mathbf{x}_{2}^{1}=\left(5+2 \mathbf{x}_{1}^{0}-2 \mathbf{x}_{3}^{0}\right) / 7=(5+0-0) / 7=0.714 \\
& \mathbf{x}_{3}^{1}=\left(1+\mathbf{x}_{1}^{0}+2 \mathbf{x}_{2}^{0}\right) / 5=(1+0+0) / 5=0.200
\end{aligned}
$$

- Second iteration (use $x^{1}$ values)

$$
\begin{aligned}
& \mathbf{x}_{1}^{2}=\left(11+2 \mathbf{x}_{2}^{1}-\mathbf{x}_{3}^{1}\right) / 6=(11+2 * 0.714-0.200) / 6=2.038 \\
& \mathbf{x}_{2}^{2}=\left(5+2 \mathbf{x}_{1}{ }^{1}-2 \mathbf{x}_{3}^{1}\right) / 7=(5+2 * 1.833-2 * 0.200) / 7=1.181 \\
& \mathbf{x}_{3}^{2}=\left(1+\mathbf{x}_{1}{ }^{1}+2 \mathbf{x}_{2}^{1}\right) / 5=(1+1.833+2 * 0.714) / 5=0.852
\end{aligned}
$$

- Continue to get

|  | Zeroth | First | Second | Third | Fourth | Fifth | $\ldots$ | Eighth |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{x}_{1}$ | 0.000 | 1.833 | 2.038 | 2.085 | 2.004 | 1.994 | $\ldots$ | 2.000 |
| $\mathrm{x}_{2}$ | 0.000 | 0.714 | 1.181 | 1.053 | 1.001 | 0.990 | $\ldots$ | 1.000 |
| $\mathrm{x}_{3}$ | 0.000 | 0.200 | 0.852 | 1.080 | 1.038 | 1.001 | $\ldots$ | 1.000 |

## Convergence of the Iterative Methods

- Note that these methods can be seen as the multiple application of Simple One-Point Iteration.
- They may converge or diverge. A convergence criteria can be derived starting from the convergence criteria of the Simple One-Point Iteration method.
- When the system of equations can be ordered so that each diagonal entry of the coefficient matrix is larger in magnitude than the sum of the magnitudes of the other coefficients in that row (diagonally dominant system) the iterations converge for any starting values. This is a sufficient but not necessary criteria.

$$
\text { For all } i=1, \ldots, n \quad\left|a_{i i}\right|>\sum_{\substack{j=1 \\ j \neq i}}^{n}\left|a_{i j}\right|
$$

- Many engineering problems satisfy this requirement.
- The example we used has a diagonally dominant coefficient matrix.
- Gauss-Seidel converges usually faster than the Jacobi method.

Exercise 14: Interchange the $2^{\text {nd }}$ and $3^{\text {rd }}$ equations of the previous example. Is the system diagonally dominant now? Solve this system using both iterative methods. Compare their convergence rates with that of the solved example. Do you observe any divergence?

## Improving Gauss-Seidel with Relaxation

- After each new value of $x$ is computed, that value is modified by a weighted average of the results of the previous and present iterations,

$$
x_{\mathbf{i}}^{\text {new }}=\lambda x_{\mathbf{i}}{ }^{\text {new }}+(1-\lambda) x_{i}{ }^{\text {old }} \quad 0<\lambda<2: \text { weighting factor }
$$

- If $\lambda=1 \rightarrow$ no relaxation (Original Gauss-Seidel)
- If $0<\lambda<1 \rightarrow$ under relaxation (Used to make a diverging system converge)
- If $1<\lambda<2 \rightarrow$ over relaxation (Used to speed up the convergence of an already converging system. Called SOR, Successive (or Simultaneous) Over Relaxation)
- Choice of $\lambda$ is problem specific.

Exercise 15: Solve the system we used in the Gauss-Seidel example with different weighting factors. Do you notice any difference in the convergence rate?

## Pseudocode for the Gauss-Seidel Method

```
LOOP k from 1 to maxIter
    LOOP i from 1 to n
        xi= Bi
        LOOP j from 1 to n
            IF (i\not=j) x i = x i - A ij }\mp@subsup{\textrm{x}}{\textrm{j}}{
    ENDLOOP
    xi= xi/ A ii
ENDLOOP
CONVERGED = TRUE
LOOP i from 1 to n
    OUTPUT xi
    \mp@subsup{\varepsilon}{a}{}}=|(\mp@subsup{x}{i}{}-\mp@subsup{x}{i}{}\mp@subsup{}{}{\mathrm{ old }})/\mp@subsup{x}{i}{\prime}|*10
    IF ( }\mp@subsup{\varepsilon}{\textrm{a}}{}>>\mathrm{ tolerance) CONVERGED = FALSE
ENDLOOP
IF (CONVERGED = TRUE) STOP
```


## Solving System of Nonlinear Equations

## Example 20: Solving a 2x2 System Using Simple One-Point Iteration

Solve the following system of equations

$$
\begin{aligned}
& x^{2}+y^{2}=4 \\
& e^{x}+y=1
\end{aligned}
$$

Put the functions into the form $x=g_{1}(x, y), y=g_{2}(x, y)$
$x=g_{1}(y)=\ln (1-y)$
$y=g_{2}(x)=-\sqrt{4-x^{2}}$


Select a starting values for $x$ and $y$, such as $x_{0}=0.0$ and $y_{0}=0.0$. They don't need to satisfy the equations. Use these values in $g$ functions to calculate new values.
$x_{1}=g_{1}\left(y_{0}\right)=0$
$y_{1}=g_{2}\left(x_{1}\right)=-2$
$x_{2}=g_{1}\left(y_{1}\right)=1.098612289$
$y_{2}=g_{2}\left(x_{2}\right)=-1.67124236$
$x_{3}=g_{1}\left(y_{2}\right)=0.982543669$
$y_{3}=g_{2}\left(x_{3}\right)=-1.74201261$
$x_{4}=g_{1}\left(y_{3}\right)=1.00869218 \quad y_{4}=g_{2}\left(x_{4}\right)=-1.72700321$
The solution is converging to the exact solution of $x=1.004169, y=-1.729637$

Exercise 18: Solve the same system but rearrange the equations as $x=\ln (1-y) \quad y=\left(4-x^{2}\right) / y$ and start from $x_{0}=1 y_{0}=-1.7$. Remember that this method may diverge.

## Solving System of Nonlinear Equations (cont’d)

## Solving a $2 \times 2$ System Using Newton-Raphson Method

Consider the following general form of a two equation system

$$
\begin{aligned}
& u(x, y)=0 \\
& v(x, y)=0
\end{aligned}
$$

Write $1^{\text {st }}$ order TSE for these equations

$$
\begin{aligned}
& u_{i+1}=u_{i}+\frac{\partial u_{i}}{\partial x}\left(x_{i+1}-x_{i}\right)+\frac{\partial u_{i}}{\partial y}\left(y_{i+1}-y_{i}\right) \\
& v_{i+1}=v_{i}+\frac{\partial v_{i}}{\partial x}\left(x_{i+1}-x_{i}\right)+\frac{\partial v_{i}}{\partial y}\left(y_{i+1}-y_{i}\right)
\end{aligned}
$$

To find the solution set $\mathbf{u}_{\mathbf{i + 1}}=0$ and $\mathrm{v}_{\mathbf{i + 1}}=0$. Rearrange

$$
\begin{aligned}
& \frac{\partial u_{i}}{\partial x} x_{i+1}+\frac{\partial u_{i}}{\partial y} y_{i+1}=-u_{i}+\frac{\partial u_{i}}{\partial x} x_{i}+\frac{\partial u_{i}}{\partial y} y_{i} \\
& \frac{\partial v_{i}}{\partial x} x_{i+1}+\frac{\partial v_{i}}{\partial y} y_{i+1}=-v_{i}+\frac{\partial v_{i}}{\partial x} x_{i}+\frac{\partial v_{i}}{\partial y} y_{i}
\end{aligned}
$$

$$
\left[\begin{array}{cc}
\frac{\partial u_{i}}{\partial x} & \frac{\partial u_{i}}{\partial y} \\
\frac{\partial v_{i}}{\partial x} & \frac{\partial v_{i}}{\partial y}
\end{array}\right]\left\{\begin{array}{l}
x_{i+1} \\
y_{i+1}
\end{array}\right\}=\left\{\begin{array}{l}
-u_{i}+\frac{\partial u_{i}}{\partial x} x_{i}+\frac{\partial u_{i}}{\partial y} y_{i} \\
-v_{i}+\frac{\partial v_{i}}{\partial x} x_{i}+\frac{\partial v_{i}}{\partial y} y_{i}
\end{array}\right\}
$$

The first matrix is called the Jacobian matrix. Solve for $\mathrm{x}_{\mathbf{i + 1}}, \mathrm{y}_{\mathrm{i+1}}$ and iterate.

Can be generalized for $n$ simultaneous equations

## Solving System of Eqns Using NR Method (cont'd)

Solve for $\mathrm{X}_{\mathrm{i}+\mathbf{1}}$ and $\mathrm{y}_{\mathrm{i+1}}$ using Cramer's rule (ME 210)
$x_{i+1}=x_{i}-\frac{u_{i} \frac{\partial v_{i}}{\partial y}-v_{i} \frac{\partial u_{i}}{\partial y}}{\frac{\partial u_{i}}{\partial x} \frac{\partial v_{i}}{\partial y}-\frac{\partial u_{i}}{\partial y} \frac{\partial v_{i}}{\partial x}} \quad, \quad y_{i+1}=y_{i}-\frac{v_{i} \frac{\partial u_{i}}{\partial x}-u_{i} \frac{\partial v_{i}}{\partial x}}{\frac{\partial u_{i}}{\partial x} \frac{\partial v_{i}}{\partial y}-\frac{\partial u_{i}}{\partial y} \frac{\partial v_{i}}{\partial x}}$

The denominator is the determinant of the Jacobian matrix $|\mathrm{J}|$.

Example 21: Solve the same system of equations

$$
\begin{aligned}
& u=x^{2}+y^{2}-4=0 \\
& v=e^{x}+y-1=0
\end{aligned} \quad \text { stating with } x_{0}=1, y_{0}=1
$$

$\frac{\partial u}{\partial x}=2 x, \frac{\partial u}{\partial y}=2 y, \frac{\partial v}{\partial x}=e^{x}, \frac{\partial v}{\partial y}=1 \rightarrow|J|=2 x-2 y e^{x}$
$x_{i+1}=x_{i}-\frac{u_{i}-2 y_{i} v_{i}}{|J|}, y_{i+1}=y_{i}-\frac{2 x v_{i}-e^{x_{i}} u_{i}}{|J|}$

| $i=0$, | $x_{0}=1$ | $y_{0}=1$ | $u_{0}=-2$ | $v_{0}=2.718282$ | $\left\|J_{0}\right\|=-3.436564$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $i=1$, | $x_{1}=-1.163953$ | $y_{1}=3.335387$ | $u_{1}=8.479595$ | $v_{1}=2.647636$ | $\left\|J_{1}\right\|=-4.410851$ |
| $i=2$, | $x_{2}=-3.245681$ | $y_{2}=1.337769$ | $u_{2}=8.324069$ | $v_{2}=0.376711$ | $\left\|J_{2}\right\|=-6.595552$ |
| $i=3$, | $x_{3}=-2.136423$ | $y_{3}=0.959110$ | $u_{3}=1.484197$ | $v_{3}=0.077187$ | $\left\|J_{3}\right\|=-4.499343$ |

Looks like it is converging to the root in the $2^{\text {nd }}$ quadrant $x \approx-1.8, y \approx 0.8$.
Exercise 19: Can you start with $\mathrm{x}_{\mathbf{0}}=0$ and $\mathrm{y}_{\mathbf{0}}=0$ ?
Exercise 20: Try to find starting points that will converge to the solution in the $4^{\text {th }}$ quadrant.

## Solving System of Nonlinear Equations (cont'd)

- Previous N-R solution of a system of 2 nonlinear equations can be generalized to the solution of a system of $n$ nonlinear equations (See page 257 for details).
- Given the following $n$ nonlinear equations with $n$ unknowns

$$
\begin{aligned}
& f_{1}\left(x_{1}, x_{2}, \ldots, x_{n}\right)=0 \\
& f_{2}\left(x_{1}, x_{2}, \ldots, x_{n}\right)=0
\end{aligned}
$$

$$
f_{n}\left(x_{1}, x_{2}, \ldots, x_{n}\right)=0
$$

- Form the Jacobian matrix.

$$
[Z]^{k}=\left[\begin{array}{cccc}
\frac{\partial f_{1}}{\partial \mathbf{x}_{1}} & \frac{\partial f_{1}}{\partial \mathbf{x}_{2}} & \cdots & \frac{\partial f_{1}}{\partial \mathbf{x}_{n}} \\
\frac{\partial f_{2}}{\partial \mathbf{x}_{1}} & \frac{\partial f_{2}}{\partial \mathbf{x}_{2}} & \cdots & \frac{\partial f_{2}}{\partial \mathbf{x}_{n}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_{n}}{\partial \mathbf{x}_{1}} & \frac{\partial f_{n}}{\partial \mathbf{x}_{2}} & \cdots & \frac{\partial f_{n}}{\partial \mathbf{x}_{n}}
\end{array}\right]^{k}
$$

k is the iteration counter.
Calculate a new [Z] at each iteration.

- Solve the following system using any of the techniques that we learned in this chapter.

$$
[Z]^{\mathbf{k}}\{x\}^{\mathbf{k}+\mathbf{1}}=-\{F\}^{\mathbf{k}}+[Z]^{\mathbf{k}}\{x\}^{\mathbf{k}} \quad \text { where } \quad F_{\mathbf{i}^{\mathbf{k}}}=\mathrm{f}_{\mathbf{i}}\left(\mathrm{X}_{1} \mathbf{k}^{\mathbf{k}}, \mathrm{x}_{2} \mathbf{k}, \ldots, \mathrm{x}_{n^{\mathbf{k}}}\right)
$$

## Example 22 (Fall 2002 Exam Question):



Link lengths:
$a_{1}=4, a_{2}=2, a_{3}=4, a_{4}=5$

Crank angle: $\quad \theta_{12}=45^{\circ}=\pi / 4$

- Use the Newton-Raphson method to solve the following set of equations for $\theta_{\mathbf{1 3}}$ and $\theta_{\mathbf{1 4}}$.
- Start with the following intial guesses: $\theta^{0}{ }_{\mathbf{1 3}}=55^{\circ}, \theta^{0}{ }_{14}=80^{\circ}$
- Perform two iterations.

$$
\begin{gathered}
f_{1}\left(\theta_{13}, \theta_{14}\right)=a_{\mathbf{2}} \cos \left(\theta_{12}\right)+a_{\mathbf{3}} \cos \left(\theta_{13}\right)-a_{4} \cos \left(\theta_{14}\right)-a_{1}=0 \\
f_{2}\left(\theta_{13}, \theta_{14}\right)=a_{\mathbf{2}} \sin \left(\theta_{12}\right)+a_{\mathbf{3}} \sin \left(\theta_{13}\right)-a_{\mathbf{4}} \sin \left(\theta_{14}\right)=0
\end{gathered}
$$

## Example 22 (cont'd)

- $\mathrm{N}-\mathrm{R}$ can be applied to nonlinear equations as follows
$[\mathrm{Z}]^{\mathbf{k}}\{\mathrm{X}\}^{\mathbf{k}+\mathbf{1}}=-\{\mathrm{F}\}^{\mathbf{k}}+[\mathrm{Z}]^{\mathbf{k}}\{X\}^{\mathbf{k}}$
where $[Z]^{\mathbf{k}}$ is the Jacobian matrix of the $\mathbf{k}^{\text {th }}$ iteration

$$
[Z]^{k}=\left[\begin{array}{ll}
\frac{\partial f_{1}}{\partial x_{1}} & \frac{\partial f_{1}}{\partial x_{2}} \\
\frac{\partial f_{2}}{\partial \mathbf{x}_{1}} & \frac{\partial f_{2}}{\partial x_{2}}
\end{array}\right]^{k}
$$

$$
\begin{array}{ll}
\frac{\partial f_{1}}{\partial x_{1}}=\frac{\partial f_{1}}{\partial \theta_{13}}=-\mathrm{a}_{3} \sin \left(\theta_{13}\right) & \frac{\partial \mathrm{f}_{1}}{\partial \mathrm{x}_{2}}=\frac{\partial \mathrm{f}_{1}}{\partial \theta_{14}}=\mathrm{a}_{4} \sin \left(\theta_{14}\right) \\
\frac{\partial \mathrm{f}_{2}}{\partial \mathrm{x}_{1}}=\frac{\partial \mathrm{f}_{2}}{\partial \theta_{13}}=\mathrm{a}_{3} \cos \left(\theta_{13}\right) & \frac{\partial \mathrm{f}_{2}}{\partial \mathrm{x}_{2}}=\frac{\partial \mathrm{f}_{2}}{\partial \theta_{14}}=-\mathrm{a}_{4} \cos \left(\theta_{14}\right)
\end{array}
$$

- Iteration $0: \theta^{0}{ }_{13}=55^{\circ}, \theta^{0} \mathbf{1 4}^{\circ}=80^{\circ}$


## Example 22 (cont'd)

- Iteration 1: $\frac{\partial f_{1}{ }^{0}}{\partial \theta_{13}}=-3.2766 \quad \frac{\partial f_{1}{ }^{0}}{\partial \theta_{14}}=4.9240 \quad \frac{\partial f_{2}{ }^{0}}{\partial \theta_{13}}=2.2943 \quad \frac{\partial f_{2}{ }^{0}}{\partial \theta_{14}}=-0.8682$

$$
[Z]^{0}=\left[\begin{array}{cc}
-3.2766 & 4.9240 \\
2.2943 & -0.8682
\end{array}\right] \quad\{F\}^{0}=\left\{\begin{array}{l}
-1.1597 \\
-0.2332
\end{array}\right\}
$$

Therefore the linear system is

$$
\left[\begin{array}{cc}
-3.2766 & 4.9240 \\
2.2943 & -0.8682
\end{array}\right]\left\{\begin{array}{l}
\theta_{13}^{1} \\
\theta_{14}^{1}
\end{array}\right\}=-\left\{\begin{array}{l}
-1.1597 \\
-0.2332
\end{array}\right\}+\left[\begin{array}{cc}
-3.2766 & 4.9240 \\
2.2943 & -0.8682
\end{array}\right]\left\{\begin{array}{l}
55 \\
80
\end{array}\right\}=\left\{\begin{array}{c}
214.8667 \\
56.9637
\end{array}\right\}
$$

Solve this system using Gauss Elimination (or any other technique that we learned) to get
$\theta^{1}{ }_{13}=55.2550^{\circ} \quad \theta^{1}{ }_{14}=80.4052^{\circ}$

## Example 22 (cont'd)

- Iteration 2: $\frac{\partial f_{1}{ }^{1}}{\partial \theta_{13}}=-3.2868 \quad \frac{\partial f_{1}{ }^{1}}{\partial \theta_{14}}=4.9301 \quad \frac{\partial f_{2}{ }^{1}}{\partial \theta_{13}}=2.2797 \quad \frac{\partial f_{2}{ }^{1}}{\partial \theta_{14}}=-0.8334$

$$
[Z]^{1}=\left[\begin{array}{cc}
-3.2868 & 4.9301 \\
2.2797 & -0.8334
\end{array}\right] \quad\{F\}^{1}=\left\{\begin{array}{c}
-1.1395 \\
-0.2291
\end{array}\right\}
$$

Therefore the linear system is

$$
\left[\begin{array}{cc}
-3.2868 & 4.9301 \\
2.2797 & -0.8334
\end{array}\right]\left\{\begin{array}{l}
\theta_{13}^{1} \\
\theta_{14}^{1}
\end{array}\right\}=-\left\{\begin{array}{l}
-1.1395 \\
-0.2291
\end{array}\right\}+\left[\begin{array}{cc}
-3.2868 & 4.9301 \\
2.2797 & -0.8334
\end{array}\right]\left\{\begin{array}{l}
55.2550 \\
80.4052
\end{array}\right\}=\left\{\begin{array}{c}
215.9330 \\
59.1842
\end{array}\right\}
$$

Solve this system using Gauss Elimination (or any other technique that we learned) to get
$\theta^{1}{ }_{13}=55.4996^{\circ} \quad \theta^{1}{ }_{14}=80.7994^{\circ}$

