## SECTION 3: SYSTEMS OF EQUATIONS

ESC 440 - Computational Methods for Engineers

## Introduction

## A System of Equations - Example


$\square$ Three masses

- $m_{1}, m_{2}$, and $m_{3}$
$\square$ Three springs
- $k_{1}, k_{2}, k_{3}$
$\square$ Connected in series and suspended
$\square$ Determine the displacement of each mass from its unstretched position


## A System of Equations - Example

Three unknown displacements: $x_{1}, x_{2}, x_{3}$

- Need three equations to find displacements
$\square$ Apply Newton's second law to each mass

$$
\begin{aligned}
& \square \text { Three equations result: } \\
& m_{1} \ddot{x}_{1}=m_{1} g+k_{2}\left(x_{2}-x_{1}\right)-k_{1} x_{1} \\
& m_{2} \ddot{x}_{2}=m_{2} g+k_{3}\left(x_{3}-x_{2}\right)-k_{2}\left(x_{2}-x_{1}\right) \\
& m_{3} \ddot{x}_{3}=m_{3} g-k_{3}\left(x_{3}-x_{2}\right)
\end{aligned}
$$

## A System of Equations - Example

$\square$ Steady-state, so $\quad \ddot{x}_{i}=0, \forall i$

$$
\begin{aligned}
& m_{1} g+k_{2}\left(x_{2}-x_{1}\right)-k_{1} x_{1}=0 \\
& m_{2} g+k_{3}\left(x_{3}-x_{2}\right)-k_{2}\left(x_{2}-x_{1}\right)=0 \\
& m_{3} g-k_{3}\left(x_{3}-x_{2}\right)=0
\end{aligned}
$$

$\square$ Rearranging

$$
\begin{array}{rr}
\left(k_{1}+k_{2}\right) x_{1} & -k_{2} x_{2}+0 x_{3}=m_{1} g \\
-k_{2} x_{1}+\left(k_{2}+k_{3}\right) x_{2}-k_{3} x_{3}=m_{2} g \\
0 x_{1}-k_{3} x_{2}+k_{3} x_{3}=m_{3} g
\end{array}
$$

## A System of Equations - Example

$\square$ Our system of three equations

$$
\begin{aligned}
& \left(k_{1}+k_{2}\right) x_{1} \\
& -k_{2} x_{2}+0 x_{3}=m_{1} g \\
& -k_{2} x_{1}+\left(k_{2}+k_{3}\right) x_{2}-k_{3} x_{3}=m_{2} g \\
& 0 x_{1} \quad-k_{3} x_{2}+k_{3} x_{3}=m_{3} g
\end{aligned}
$$

can be put into matrix form

$$
\left[\begin{array}{ccc}
\left(k_{1}+k_{2}\right) & -k_{2} & 0 \\
-k_{2} & \left(k_{2}+k_{3}\right) & -k_{3} \\
0 & -k_{3} & k_{3}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{c}
m_{1} g \\
m_{2} g \\
m_{3} g
\end{array}\right]
$$

## A System of Equations - Example

$$
\left[\begin{array}{ccc}
\left(k_{1}+k_{2}\right) & -k_{2} & 0 \\
-k_{2} & \left(k_{2}+k_{3}\right) & -k_{3} \\
0 & -k_{3} & k_{3}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
m_{1} g \\
m_{2} g \\
m_{3} g
\end{array}\right]
$$

$\square$ We can rewrite this matrix equation as

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

$\square$ Can apply tools of linear algebra to determine the vector of unknown displacements

$$
\mathbf{x}=\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]
$$

## Matrix notation

Conventions for matrix notation vary greatly. In general, the dimensions of a variable are known from context. These notes will use the following convention:
$\square$ Matrices

- Upper-case, bold variables, e.g. A
$\square$ Vectors
- Lower-case, bold variables, e.g. x
$\square$ Hand-written matrices and vectors
- Underbar, instead of bold, e.g. $\underline{A}$ or $\underline{x}$


## Solving Systems of Equations with Python

Before getting into the algorithms used to solve systems of linear equations, we'll take a look at how we can use available Python functions to find a solution.

## System as a Matrix Equation

$\square$ Our system of equations has the form

$$
\begin{aligned}
& a_{11} x_{1}+a_{12} x_{2}+a_{13} x_{3}=b_{1} \\
& a_{21} x_{1}+a_{22} x_{2}+a_{23} x_{3}=b_{2} \\
& a_{31} x_{1}+a_{32} x_{2}+a_{33} x_{3}=b_{3}
\end{aligned}
$$

$\square$ This can be written in matrix form as

$$
\left[\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
b_{1} \\
b_{2} \\
b_{3}
\end{array}\right]
$$

or

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

## Solving the Matrix Equation

$\square$ Solving our system of equations amounts to solving the matrix equation

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

for the vector $\mathbf{x}$
$\square$ To isolate $\mathbf{x}$ on the left of the equal sign, left multiply by the inverse of the coefficient matrix

$$
\begin{gathered}
A^{-1} A x=A^{-1} b \\
x=A^{-1} b
\end{gathered}
$$

## Solving the Matrix Equation

$\square$ In NumPy's linalg module - left-multiply by $\mathbf{A}^{\mathbf{1}}$

```
# %% solve using matrix inverse
import numpy as np
A = np.array([[7, 3, 8],
    [2, 1, 9],
b = np.array([3, 7, 2])
x = np.linalg.inv(A)@b
print('\n x =', x)
```

$\square$ Use np.linalg.inv() for matrix inversion
$\square$ Use @ for matrix multiplication

-     * performs element-by-element multiplication
$\square$ Note that b can be a row or column vector
- Treated as a column vector either way
$\square$ Matrix inversion works, but is not always the best way to solve
- Inefficient, slow
- Sensitive to numerical error
- Some systems worse than others


## Solving the Matrix Equation

$\square$ Instead, use NumPy's linalg. solve( ) function


In [5]: runcell('solve using np.linalg.solve', Notes/Python/Section3/linSysSolve.py')
$x=\left[\begin{array}{lll}-0.50359712 & -0.28057554 & 0.92086331\end{array}\right]$
$\square$ If $\mathbf{A}^{\mathbf{1}}$ exists, then

$$
x=n p . l i n a l g . s o l v e(A, b)
$$

is equivalent to

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

$\square$ Does not calculate $\mathbf{A}^{\mathbf{- 1}}$

- Faster, more robust
$\square$ Makes use of techniques we'll explore next


## Example - Solving Using NumPy


$\square$ Our linear system is described by the matrix equation

$$
\begin{gathered}
{\left[\begin{array}{ccc}
\left(k_{1}+k_{2}\right) & -k_{2} & 0 \\
-k_{2} & \left(k_{2}+k_{3}\right) & -k_{3} \\
0 & -k_{3} & k_{3}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{c}
m_{1} g \\
m_{2} g \\
m_{3} g
\end{array}\right]} \\
\mathbf{A x}=\mathbf{b}
\end{gathered}
$$

Find the displacements, $\mathbf{x}$, for the following system parameters

- $k_{1}=500 \frac{\mathrm{~N}}{\mathrm{~m}}, k_{2}=800 \frac{\mathrm{~N}}{\mathrm{~m}}, k_{3}=400 \frac{\mathrm{~N}}{\mathrm{~m}}$

口 $m_{1}=3 \mathrm{~kg}, m_{2}=1 \mathrm{~kg}, m_{3}=7 \mathrm{~kg}$

## Example - Solving Using NumPy



$$
x_{1}=21.6 \mathrm{~cm}, \quad x_{2}=31.4 \mathrm{~cm}, \quad x_{3}=48.6 \mathrm{~cm}
$$

## Solving Systems of Linear Equations

$\square$ Techniques exist for finding the solution to small systems of linear equations:

- Graphical method
- Cramer's rule
- Elimination of unknowns
$\square$ Not generally useful for numerical solution of larger systems, but they do provide insight
$\square$ For numerical solution of larger systems techniques include:
- Gaussian elimination
- Jacobi method
- Gauss-Seidel


## Graphical Solution

$\square$ A system of two linear equations with two unknown variables

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

can be thought of as equations of two lines in the $x-y$ plane:

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

## Graphical Solution

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

$\square$ Solution to this system of equations is the point of intersection $\left(x_{1}, x_{2}\right)$ of the two lines

- May not exist
$\square$ May not be unique
$\square$ May exist, but be difficult to determine accurately


## Unique Solution

$\square$ System of two linear equations:

$$
\begin{array}{r}
0.5 x_{1}+x_{2}=5 \\
3 x_{1}-x_{2}=2
\end{array}
$$

$\square$ Represented in matrix form

$$
\begin{gathered}
{\left[\begin{array}{cc}
0.5 & 1 \\
3 & -1
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]=\left[\begin{array}{l}
5 \\
2
\end{array}\right]} \\
\mathbf{A} \mathbf{x}=\mathbf{b}
\end{gathered}
$$

Unique Solution

$\square$ Solution at the point of intersection: $\left(x_{1}, x_{2}\right)=(2,4)$

## No Solution

$\square$ System of two linear equations:

$$
\begin{aligned}
& 3 x_{1}-x_{2}=2 \\
& 3 x_{1}-x_{2}=4
\end{aligned}
$$

$\square$ Represented in matrix form

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

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


$\square$ Lines don't intersect, so no solution exists

## Infinite Solutions

$\square$ System of two linear equations:

$$
\begin{aligned}
3 x_{1}-x_{2} & =2 \\
-6 x_{1}+2 x_{2} & =-4
\end{aligned}
$$

$\square$ Represented in matrix form

$$
\begin{gathered}
{\left[\begin{array}{cc}
3 & -1 \\
-6 & 2
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]=\left[\begin{array}{c}
2 \\
-4
\end{array}\right]} \\
\mathbf{A x}=\mathbf{b}
\end{gathered}
$$

Infinite Number of Solutions

$\square$ Solutions at all points along the lines

## III-Conditioned System

$\square$ System of two linear equations:

$$
\begin{gathered}
0.5 x_{1}+x_{2}=5 \\
0.48 x_{1}+x_{2}=4.96
\end{gathered}
$$

$\square$ Represented in matrix form

$$
\begin{gathered}
{\left[\begin{array}{cc}
0.5 & 1 \\
0.48 & 1
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]=\left[\begin{array}{c}
5 \\
4.96
\end{array}\right]} \\
\mathbf{A x}=\mathbf{b}
\end{gathered}
$$


$\square$ Solutions exists, but it is difficult to identify accurately

## Singularity and the Coefficient Matrix, A

$\square$ Systems with no solutions or infinite solutions are both referred to as singular
$\square$ Coefficient matrix, $\mathbf{A}$, is singular

- $\mathbf{A}^{\mathbf{1}}$, does not exist
$\square \operatorname{det}(\mathbf{A})=0$
$\square$ For the example with no solutions

$$
\operatorname{det}(\mathbf{A})=\left|\begin{array}{ll}
3 & -1 \\
3 & -1
\end{array}\right|=-3-(-3)=0
$$

$\square$ For the example with infinite solutions

$$
\operatorname{det}(\mathbf{A})=\left|\begin{array}{cc}
3 & -1 \\
-6 & 2
\end{array}\right|=6-6=0
$$

## III-Conditioned Systems

$\square$ III-conditioned systems are nearly-singular
$\square \operatorname{det}(\mathbf{A}) \approx 0$
$\square \mathbf{A}^{\mathbf{1}}$ exists, but may be difficult to determine accurately
$\square$ Solution exists, but it may difficult to determine accurately - either graphically or numerically
$\square$ For the previous example of an ill-conditioned system

$$
\operatorname{det}(\mathbf{A})=\left|\begin{array}{cc}
0.5 & 1 \\
0.48 & 1
\end{array}\right|=0.5-0.48=0.02
$$

(This example may be ill-conditioned for graphical solution, but would not be if solving numerically)

## Rank of the Coefficient Matrix, A

$\square$ Rank of a matrix - number of linearly-independent rows (or columns) of the matrix
$\square$ Full-rank matrix

- All rows and columns are linearly-independent
- Must be square
$\square \operatorname{det}(\mathbf{A}) \neq 0, \mathbf{A}^{\mathbf{1}}$ exists
$\square$ In both of our singular examples $\mathbf{A}$ is rank-deficient

$$
\mathbf{A}_{\mathbf{1}}=\left[\begin{array}{ll}
3 & -1 \\
3 & -1
\end{array}\right] \quad \text { and } \quad \mathbf{A}_{2}=\left[\begin{array}{cc}
3 & -1 \\
-6 & 2
\end{array}\right]
$$

$\square$ For a $2 \times 2$, rank-deficient matrix, columns and rows represent collinear vectors

# Gaussian Elimination 

## Gaussian Elimination

$\square$ Two steps in Gaussian elimination:

- Elimination of unknowns
- Solution through back-substitution
$\square$ Applies to arbitrarily large systems

$$
\begin{gathered}
a_{11} x_{1}+a_{12} x_{2}+\cdots+a_{1 n} x_{n}=b_{1} \\
a_{21} x_{1}+a_{22} x_{2}+\cdots+a_{2 n} x_{n}=b_{2} \\
\vdots \\
\vdots \\
a_{n 1} x_{1}+a_{n 2} x_{2}+\cdots+a_{n n} x_{n}=b_{n}
\end{gathered}
$$

$\square$ The basic algorithm will be introduced using an example system of three equations with three unknowns

## Gaussian Elimination - the Basic Algorithm

$\square$ The basic algorithm:

1. Forward elimination of unknowns

- Reduce to an upper-triangular system

2. Back-substitution to solve for unknowns

- Reduction to an upper-triangular system yields the solution for $x_{n}$ directly
- Back-substitute the solution for $x_{n}$ to solve for $x_{n-1}$
- Back-substitute the solution for $x_{n-1}$ to solve for $x_{n-2}$
- Continue until all $x_{i}$ have been determined


## Forward Elimination of Unknowns

$\square$ We'll use a system of three equations with three unknowns as an example

$$
\left[\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{l}
b_{1} \\
b_{2} \\
b_{3}
\end{array}\right]
$$

$\square$ Create the augmented system matrix

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
a_{21} & a_{22} & a_{23} & \vdots & b_{2} \\
a_{31} & a_{32} & a_{33} & \vdots & b_{3}
\end{array}\right]
$$

$\square$ Each row represents an equation - row operations are operations on the equations

## Forward Elimination of Unknowns

$\square$ Reduce to an upper-triangular system
$\square$ Eliminate $x_{i}$ from the $(i+1)^{\text {st }}$ through $n^{\text {th }}$ equations for $i=1 \ldots n$
$\square$ First eliminate $x_{1}$ from the second equation

- Perform row operations to set the first element on the second row to zero
- Normalize the first equation (row) - divide by the leading coefficient, $a_{11}$
- Multiply the first equation (row) by the leading coefficient of the second equation (row), $a_{21}$

$$
\left[\begin{array}{ccccc}
a_{21} & \frac{a_{21}}{a_{11}} a_{12} & \frac{a_{21}}{a_{11}} a_{13} & \vdots & \frac{a_{21}}{a_{11}} b_{1} \\
a_{21} & a_{22} & a_{23} & \vdots & b_{2} \\
a_{31} & a_{32} & a_{33} & \vdots & b_{3}
\end{array}\right]
$$

## Forward Elimination of Unknowns

$\square$ Subtract the first row from the second, and replace the first row with its original values

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}-\frac{a_{21}}{a_{11}} a_{12} & a_{23}-\frac{a_{21}}{a_{11}} a_{13} & \vdots & b_{2}-\frac{a_{21}}{a_{11}} b_{1} \\
a_{31} & a_{32} & a_{33} & \vdots & b_{3}
\end{array}\right]
$$

$\square$ Use prime notation to indicate a modified coefficient value

- Add additional prime mark for each modification

$$
\left[\begin{array}{cllll}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
a_{31} & a_{32} & a_{33} & \vdots & b_{3}
\end{array}\right]
$$

## Forward Elimination of Unknowns

$\square$ Next, eliminate $x_{1}$ from the third equation

- Normalize the first row
- Multiply by the leading coefficient of the third row, $a_{31}$

$$
\left[\begin{array}{ccccc}
a_{31} & \frac{a_{31}}{a_{11}} a_{12} & \frac{a_{31}}{a_{11}} a_{13} & \vdots & \frac{a_{31}}{a_{11}} b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
a_{31} & a_{32} & a_{33} & \vdots & b_{3}
\end{array}\right]
$$

- Subtract the first row from the third and reset the first row to its original values

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
0 & a_{32}-\frac{a_{31}}{a_{11}} a_{12} & a_{33}-\frac{a_{31}}{a_{11}} a_{13} & \vdots & b_{3}-\frac{a_{31}}{a_{11}} b_{1}
\end{array}\right]=\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
0 & a_{32}^{\prime} & a_{33}^{\prime} & \vdots & b_{3}^{\prime}
\end{array}\right]
$$

## Elimination of Unknowns - Terminology

$\square$ First row is used for the elimination of $x_{1}$ from second and third rows
$\square$ In general, $i^{\text {th }}$ row used to eliminate the $i^{\text {th }}$ unknown from the $(i+1)^{\text {st }}$ through $n^{\text {th }}$ rows

- This is the pivot row
$\square(n-1)$ rows will be pivot rows at some point
$\square$ Leading coefficient in the pivot row, $a_{i i}$, is the pivot element
$\square$ Normalization involves dividing the pivot row by the pivot element
$\square$ Could this be problematic?


## Forward Elimination of Unknowns

$\square$ Finally, eliminate $x_{2}$ from the third equation

- Normalize the second row (the pivot row)
$\square$ Multiply by the leading coefficient of the third row, $a_{32}^{\prime}$

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{32}^{\prime} & \frac{a_{32}^{\prime}}{a_{22}^{\prime}} a_{23}^{\prime} & \vdots & \frac{a_{32}^{\prime}}{a_{22}^{\prime}} b_{2}^{\prime} \\
0 & a_{32}^{\prime} & a_{33}^{\prime} & \vdots & b_{3}^{\prime}
\end{array}\right]
$$

$\square$ Subtract the second row from the third and reset the second row to its previous values

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
0 & 0 & a_{33}^{\prime}-\frac{a_{32}^{\prime 3}}{a_{22}^{\prime}} a_{23}^{\prime} & : & b_{3}^{\prime}-\frac{a_{32}^{\prime}}{a_{22}^{\prime}} b_{2}^{\prime}
\end{array}\right]=\left[\begin{array}{ccc:c}
a_{11} & a_{12} & a_{13} & \vdots \\
0 & b_{22}^{\prime} & a_{13}^{\prime} & \vdots \\
0 & 0 & a_{33}^{\prime 3} & : \\
b_{3}^{\prime \prime}
\end{array}\right]
$$

## Back-Substitution

$\square$ System is now upper-triangular

$$
\left[\begin{array}{ccccc}
a_{11} & a_{12} & a_{13} & \vdots & b_{1} \\
0 & a_{22}^{\prime} & a_{23}^{\prime} & \vdots & b_{2}^{\prime} \\
0 & 0 & a_{33}^{\prime \prime} & \vdots & b_{3}^{\prime \prime}
\end{array}\right]
$$

$\square$ Last row represents a single equation with a single unknown, $x_{3}$

$$
x_{3}=\frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}
$$

$\square$ In general, solve for the $n^{t h}$ unknown as

$$
x_{n}=\frac{b_{n}^{(n-1)}}{a_{n n}^{(n-1)}}
$$

## Back-Substitution

$\square$ Next, substitute $x_{3}$ into the second equation

$$
\begin{gathered}
a_{22}^{\prime} x_{2}+a_{23}^{\prime} x_{3}=b_{2}^{\prime} \\
a_{22}^{\prime} x_{2}+a_{23}^{\prime} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}=b_{2}^{\prime}
\end{gathered}
$$

and solve for $x_{2}$

$$
x_{2}=\frac{b_{2}^{\prime}-a_{23}^{\prime} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}}{a_{22}^{\prime}}
$$

$\square$ In general:

$$
x_{i}=\frac{1}{a_{i i}^{(i-1)}}\left(b_{i}^{(i-1)}-\sum_{j=i+1}^{n} a_{i j}^{(i-1)} x_{j}\right)
$$

## Back-Substitution

$\square$ Finally, substitute $x_{2}$ and $x_{3}$ into the first equation

$$
\begin{gathered}
a_{11} x_{1}+a_{12} x_{2}+a_{13} x_{3}=b_{1} \\
a_{11} x_{1}+a_{12} \frac{b_{2}^{\prime}-a_{23}^{\prime} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}}{a_{22}^{\prime}}+a_{13} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}=b_{1}
\end{gathered}
$$

and solve for $x_{1}$

$$
x_{1}=\frac{b_{1}-a_{12} \frac{b_{2}^{\prime}-a_{23}^{\prime} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}}{a_{22}^{\prime}}-a_{13} \frac{b_{3}^{\prime \prime}}{a_{33}^{\prime \prime}}}{a_{11}}
$$

$\square \quad$ In practice we'd solve for $x_{1}$ using the general formula

$$
x_{i}=\frac{1}{a_{i i}^{(i-1)}}\left(b_{i}^{(i-1)}-\sum_{j=i+1}^{n} a_{i j}^{(i-1)} x_{j}\right)
$$

## Algorithm Summary

1) Form augmented system matrix
2) Elimination of unknowns - for $i=1 \ldots n-1$
a) Normalize pivot row ( $i^{\text {th }}$ row)
b) Multiply pivot row by leading coefficient of $j^{\text {th }}$ row, $a_{j i}$ (for $j=(i+1) \ldots n$ )
c) Subtract pivot row from $j^{\text {th }}$ row
3) Back-substitution
a) Determine $x_{n}$ from the last row: $x_{n}=\frac{b_{n}^{(n-1)}}{a_{n n}^{(n-1)}}$
b) Solve for remaining $x_{i}$ for $i=(n-1) \ldots 1$ :

$$
x_{i}=\frac{1}{a_{i i}^{(i-1)}}\left(b_{i}^{(i-1)}-\sum_{j=i+1}^{n} a_{i j}^{(i-1)} x_{j}\right)
$$

## Partial Pivoting

$\square$ During forward elimination of unknowns, pivot row is normalized
$\square i^{\text {th }}$ row divided by leading coefficient, $a_{i i}$

- If $a_{i i}=0 \rightarrow$ divide-by-zero, algorithm fails
- If $a_{i i} \approx 0 \rightarrow$ not fatal, but susceptible to roundoff error
$\square$ Partial pivoting
$\square$ Prior to normalizing the pivot $\left(i^{\text {th }}\right)$ row, search all rows from $i \ldots n$ for the one with the largest value in the $i^{t h}$ column
$\square$ Move to the current pivot row location and continue with algorithm


# Gaussian Elimination - Example 

## Example - Truss Analysis

$\square$ Simple statically-determinate truss
$\square$ Determine all internal and external forces


## Example - Truss Analysis

## $\square$ Force components at each joint must balance



$$
\begin{aligned}
& F_{A x}+F_{A C}+F_{A B} \cos \left(55^{\circ}\right)=0 \\
& F_{A y}+F_{A B} \sin \left(55^{\circ}\right)=0
\end{aligned}
$$

$$
\begin{aligned}
& -F_{A C}-F_{B C} \cos \left(35^{\circ}\right)=0 \\
& F_{C y}+F_{B C} \sin \left(35^{\circ}\right)=0
\end{aligned}
$$

## Example - Truss Analysis

$\square$ System of six equations with six unknown internal and external forces

$$
\left[\begin{array}{cccccc}
\cos \left(55^{\circ}\right) & 1 & 0 & 1 & 0 & 0 \\
\sin \left(55^{\circ}\right) & 0 & 0 & 0 & 1 & 0 \\
-\cos \left(55^{\circ}\right) & 0 & \cos \left(35^{\circ}\right) & 0 & 0 & 0 \\
\sin \left(55^{\circ}\right) & 0 & \sin \left(35^{\circ}\right) & 0 & 0 & 0 \\
0 & -1 & -\cos \left(35^{\circ}\right) & 0 & 0 & 0 \\
0 & 0 & \sin \left(35^{\circ}\right) & 0 & 0 & 1
\end{array}\right]\left[\begin{array}{l}
F_{A B} \\
F_{A C} \\
F_{B C} \\
F_{A x} \\
F_{A y} \\
F_{C y}
\end{array}\right]=\left[\begin{array}{c}
0 \\
0 \\
0 \\
-4000 \\
0 \\
0
\end{array}\right]
$$

$\square$ Python Gaussian elimination demo...

## Example - Truss Analysis

```
# truss_example.py
import numpy as np
from gausselim import gausselim
theta1 = np.radians(55)
theta2 = np.radians(35)
A = np.array([[np.cos(theta1), 1,
    [np.sin(theta1), 0,
    [-np.cos(theta1), 0,
b = np.array([0, 0, 0, -4e3, 0, 0])
x = np.linalg.solve(A, b)
x = gausselim(A,b)
print('\n x = \n', x)
```

    [np.sin(theta1), 0, np.sin(theta2), 0, 0, 0],
    [0, -1, -np.cos(theta2), 0, 0, 0],
    \([0, \quad 0\), np.sin(theta2), 0, 0, 1]])
    

$$
\begin{array}{ll}
F_{A B}=-3.277 \mathrm{kN} & F_{A x}=0 \mathrm{~N} \\
F_{A C}=1.879 \mathrm{kN} & F_{A y}=2.684 \mathrm{kN} \\
F_{B C}=-2.294 \mathrm{kN} & F_{C y}=1.316 \mathrm{kN}
\end{array}
$$

```
In [42]: runfile('C:/Users
wdir='C:/Users/webbky/Box/
Reloaded modules: gausseli
x =
    [[-3276.60817716]
    [ 1879.38524157]
    [-2294.3057454 ]
[ 0.
[ 2684.04028665]
[ 1315.95971335]]
In [43]:
```


## Gaussian Elimination

$\square$ Gaussian elimination summary:

- Create the augmented system matrix
- Forward elimination
- Reduce to an upper-triangular matrix
- Back substitution
- Starting with $x_{N}$, solve for $x_{i}$ for $i=N \ldots 1$
$\square$ A direct solution algorithm
- Exact value for each $x_{i}$ arrived at with a single execution of the algorithm
$\square$ Alternatively, we can use an iterative algorithm
$\square$ Jacobi method
- Gauss-Seidel
- Newton-Raphson

Linear Systems of Equations Iterative Solution - Jacobi Method

## Jacobi Method

$\square$ Consider a system of $N$ linear equations

$$
\begin{gathered}
\mathbf{A} \cdot \mathbf{x}=\mathbf{y} \\
{\left[\begin{array}{ccc}
a_{1,1} & \cdots & a_{1, N} \\
\vdots & \ddots & \vdots \\
a_{N, 1} & \cdots & a_{N, N}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{N}
\end{array}\right]=\left[\begin{array}{c}
y_{1} \\
\vdots \\
y_{N}
\end{array}\right]}
\end{gathered}
$$

$\square$ The $k^{\text {th }}$ equation ( $k^{\text {th }}$ row) is

$$
\begin{equation*}
a_{k, 1} x_{1}+a_{k, 2} x_{2}+\cdots+a_{k, k} x_{k}+\cdots+a_{k, N} x_{N}=y_{k} \tag{1}
\end{equation*}
$$

$\square$ Solve (1) for $x_{k}$

$$
\begin{array}{r}
x_{k}=\frac{1}{a_{k, k}}\left[y_{k}-\left(a_{k, 1} x_{1}+a_{k, 2} x_{2}+\cdots+a_{k, k-1} x_{k-1}+\right.\right.  \tag{2}\\
\\
\left.\left.+a_{k, k+1} x_{k+1}+\cdots+a_{k, N} x_{N}\right)\right]
\end{array}
$$

## Jacobi Method

$\square$ Simplify (2) using summing notation

$$
\begin{equation*}
x_{k}=\frac{1}{a_{k, k}}\left[y_{k}-\sum_{n=1}^{k-1} a_{k, n} x_{n}-\sum_{n=k+1}^{N} a_{k, n} x_{n}\right], \quad k=1 \ldots N \tag{3}
\end{equation*}
$$

$\square$ An equation for $x_{k}$

- But, of course, we don't yet know all other $x_{n}$ values
$\square$ Use (3) as an iterative expression

$$
\begin{equation*}
x_{k, i+1}=\frac{1}{a_{k, k}}\left[y_{k}-\sum_{n=1}^{k-1} a_{k, n} x_{n, i}-\sum_{n=k+1}^{N} a_{k, n} x_{n, i}\right], \quad k=1 \ldots N \tag{4}
\end{equation*}
$$

$\square$ The $i$ subscript indicates iteration number
$\square x_{k, i+1}$ is the updated value from the current iteration

- $x_{n, i}$ is a value from the previous iteration


## Jacobi Method

$$
\begin{equation*}
x_{k, i+1}=\frac{1}{a_{k, k}}\left[y_{k}-\sum_{n=1}^{k-1} a_{k, n} x_{n, i}-\sum_{n=k+1}^{N} a_{k, n} x_{n, i}\right], \quad k=1 \ldots N \tag{4}
\end{equation*}
$$

$\square$ Old values of $x_{n}$, on the right-hand side, are used to update $x_{k}$ on the left-hand side
$\square$ Start with an initial guess for all unknowns, $\mathbf{x}_{0}$
$\square$ Iterate until adequate convergence is achieved

- Until a specified stopping criterion is satisfied
$\square$ Convergence is not guaranteed


## Convergence

$\square$ An approximation of $\mathbf{x}$ is refined on each iteration
$\square$ Continue to iterate until we're close to the right answer for the vector of unknowns, $\mathbf{x}$

- Assume we've converged to the right answer when $\mathbf{x}$ changes very little from iteration to iteration
$\square$ On each iteration, calculate a relative error quantity

$$
\varepsilon_{i+1}=\max \left(\left|\frac{x_{k, i+1}-x_{k, i}}{x_{k, i+1}}\right|\right), \quad k=1 \ldots N
$$

$\square$ Iterate until

$$
\varepsilon_{i} \leq \varepsilon_{s}
$$

where $\varepsilon_{s}$ is a chosen stopping criterion

## Jacobi Method - Matrix Form

$\square$ The Jacobi method iterative formula, (4), can be rewritten in matrix form:

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{M} \mathbf{x}_{i}+\mathbf{D}^{-1} \mathbf{y} \tag{5}
\end{equation*}
$$

where $\mathbf{D}$ is the diagonal elements of $\mathbf{A}$

$$
\mathbf{D}=\left[\begin{array}{cccc}
a_{1,1} & 0 & \cdots & 0 \\
0 & a_{2,2} & 0 & \vdots \\
\vdots & 0 & \ddots & 0 \\
0 & \cdots & 0 & a_{N, N}
\end{array}\right]
$$

and

$$
\begin{equation*}
\mathbf{M}=\mathbf{D}^{-1}(\mathbf{D}-\mathbf{A}) \tag{6}
\end{equation*}
$$

- Recall that the inverse of a diagonal matrix is given by inverting each diagonal element

$$
\mathbf{D}^{\boldsymbol{- 1}}=\left[\begin{array}{cccc}
1 / a_{1,1} & 0 & \cdots & 0 \\
0 & 1 / a_{2,2} & 0 & \vdots \\
\vdots & 0 & \ddots & 0 \\
0 & \cdots & 0 & 1 / a_{N, N}
\end{array}\right]
$$

## Jacobi Method - Example

$\square$ Consider the following system of equations

$$
\begin{aligned}
& -4 x_{1}+7 x_{3}=-5 \\
& 2 x_{1}-3 x_{2}+5 x_{3}=-12 \\
& x_{2}-3 x_{3}=3
\end{aligned}
$$

$\square$ In matrix form:

$$
\left[\begin{array}{ccc}
-4 & 0 & 7 \\
2 & -3 & 5 \\
0 & 1 & -3
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=\left[\begin{array}{c}
-5 \\
-12 \\
3
\end{array}\right]
$$

$\square$ Solve using the Jacobi method

## Jacobi Method - Example

$\square$ The iteration formula is

$$
\mathbf{x}_{i+1}=\mathbf{M} \mathbf{x}_{i}+\mathbf{D}^{-1} \mathbf{y}
$$

where

$$
\begin{aligned}
& \mathbf{D}= {\left[\begin{array}{ccc}
-4 & 0 & 0 \\
0 & -3 & 0 \\
0 & 0 & -3
\end{array}\right] \quad \mathbf{D}^{-1}=\left[\begin{array}{cc}
-0.25 & 0 \\
0 & -0.333 \\
0 & 0
\end{array}\right.} \\
& \mathbf{M}=\mathbf{D}^{-1}(\mathbf{D}-\mathbf{A})=\left[\begin{array}{ccc}
0 & 0 & 1.75 \\
0.667 & 0 & 1.667 \\
0 & 0.333 & 0
\end{array}\right]
\end{aligned}
$$

$\square$ To begin iteration, we need a starting point

- Initial guess for unknown values, $\mathbf{x}$
- Often, we have some idea of the answer
- Here, arbitrarily choose

$$
\mathbf{x}_{0}=\left[\begin{array}{lll}
10 & 25 & 10
\end{array}\right]^{T}
$$

## Jacobi Method - Example

$\square$ At each iteration, calculate

$$
\begin{gathered}
\mathbf{x}_{i+1}=\mathbf{M} \mathbf{x}_{i}+\mathbf{D}^{-1} \mathbf{y} \\
{\left[\begin{array}{l}
x_{1, i+1} \\
x_{2, i+1} \\
x_{3, i+1}
\end{array}\right]=\left[\begin{array}{ccc}
0 & 0 & 1.75 \\
0.667 & 0 & 1.667 \\
0 & 0.333 & 0
\end{array}\right]\left[\begin{array}{l}
x_{1, i} \\
x_{2, i} \\
x_{3, i}
\end{array}\right]+\left[\begin{array}{c}
1.25 \\
4 \\
-1
\end{array}\right]}
\end{gathered}
$$

$\square$ For $i=0$ :

$$
\begin{aligned}
& \mathbf{x}_{1}=\left[\begin{array}{l}
x_{1,1} \\
x_{2,1} \\
x_{3,1}
\end{array}\right]=\left[\begin{array}{ccc}
0 & 0 & 1.75 \\
0.667 & 0 & 1.667 \\
0 & 0.333 & 0
\end{array}\right]\left[\begin{array}{l}
10 \\
25 \\
10
\end{array}\right]+\left[\begin{array}{c}
1.25 \\
4 \\
-1
\end{array}\right] \\
& \mathbf{x}_{1}=\left[\begin{array}{lll}
18.75 & 27.33 & 7.33
\end{array}\right]^{T}
\end{aligned}
$$

$\square$ The relative error is

$$
\varepsilon_{1}=\max \left(\left|\frac{x_{k, 1}-x_{k, 0}}{x_{k, 1}}\right|\right)=0.467
$$

## Jacobi Method - Example

$\square$ For $i=1$ :

$$
\begin{aligned}
& \mathbf{x}_{2}=\left[\begin{array}{l}
x_{1,2} \\
x_{2,2} \\
x_{3,2}
\end{array}\right]=\left[\begin{array}{ccc}
0 & 0 & 1.75 \\
0.667 & 0 & 1.667 \\
0 & 0.333 & 0
\end{array}\right]\left[\begin{array}{c}
18.75 \\
27.33 \\
7.33
\end{array}\right]+\left[\begin{array}{c}
1.25 \\
4 \\
-1
\end{array}\right] \\
& \mathbf{x}_{2}=\left[\begin{array}{lll}
14.08 & 28.72 & 8.11
\end{array}\right]^{T}
\end{aligned}
$$

$\square$ The relative error is

$$
\varepsilon_{2}=\max \left(\left|\frac{x_{k, 2}-x_{k, 1}}{x_{k, 1}}\right|\right)=0.331
$$

$\square$ Continue to iterate until relative error falls below a specified stopping condition

## Jacobi Method - Example

$\square$ Automate with computer code, e.g. Python
$\square$ Setup the system of equations

```
77
```

```
# coefficient matrix
A = np.array([[-4, 0, 7],
    [2, -3, 5],
    [0, 1, -3]])
# vector of knowns
y = np.array([-5, -12, 3])
```

$\square$ Initialize matrices and parameters for iteration

```
17 reltol = 1e-6
18 eps = 1
19
max_iter = 600
iter = 0
# initial guess for }
x = np.array([10, 25, 10])
D = np.diag(np.diag(A))
invD = np.linalg.inv(D)
M = invD@(D - A)
```


## Jacobi Method - Example

$\square$ Loop to continue iteration as long as:

- Stopping criterion is not satisfied
- Maximum number of iterations is not exceeded

```
33
```

while((eps > reltol) and (iter < max_iter)):
xold $=x$
$x=M @ x o l d+i n v D @ y$
eps $=n p \cdot \max (a b s((x-x o l d) / x))$
iter = iter + 1
$\square$ On each iteration

- Use previous $\mathbf{x}$ values to update $\mathbf{x}$
- Calculate relative error
- Increment the number of iterations


## Jacobi Method - Example

$\square$ Set $\varepsilon_{s}=1 \times 10^{-6}$ and iterate:

| $\boldsymbol{i}$ | $\mathbf{x}_{\boldsymbol{i}}$ |  |  |
| :---: | :---: | :---: | :---: |
| 0 | $\left[\begin{array}{lll}10 & 25 & 10\end{array}\right]^{T}$ | $\varepsilon_{i}$ |  |
| 1 | $\left[\begin{array}{lll}18.75 & 27.33 & 7.33\end{array}\right]^{T}$ | 0.467 |  |
| 2 | $\left[\begin{array}{lll}14.08 & 28.72 & 8.11\end{array}\right]^{T}$ | 0.331 |  |
| 3 | $\left[\begin{array}{lll}15.44 & 26.91 & 8.57\end{array}\right]^{T}$ | 0.088 |  |
| 4 | $\left[\begin{array}{lll}16.25 & 28.59 & 7.97\end{array}\right]^{T}$ | 0.076 |  |
| 5 | $\left[\begin{array}{lll}15.20 & 28.12 & 8.53\end{array}\right]^{T}$ | 0.070 |  |
| 6 | $\left[\begin{array}{lll}16.18 & 28.35 & 8.37\end{array}\right]^{T}$ | 0.061 |  |
| $\vdots$ |  | $\vdots$ |  |
| 371 | $\left[\begin{array}{lll}20.50 & 36.00 & 11.00\end{array}\right]^{T}$ | $0.995 \times 10^{-6}$ |  |

$\square$ Convergence achieved in 371 iterations

Linear Systems of Equations Iterative Solution - Gauss-Seidel

## Gauss-Seidel Method

$\square$ The iterative formula for the Jacobi method is

$$
\begin{equation*}
x_{k, i+1}=\frac{1}{a_{k, k}}\left[y_{k}-\sum_{n=1}^{k-1} a_{k, n} x_{n, i}-\sum_{n=k+1}^{N} a_{k, n} x_{n, i}\right], \quad k=1 \ldots N \tag{4}
\end{equation*}
$$

$\square$ Note that only old values of $x_{n}$ (i.e. $x_{n, i}$ ) are used to update the value of $x_{k}$
$\square$ Assume the $x_{k, i+1}$ values are determined in order of increasing $k$

- When updating $x_{k, i+1}$, all $x_{n, i+1}$ values are already known for $n<k$
- We can use those updated values to calculate $x_{k, i+1}$
- The Gauss-Seidel method


## Gauss-Seidel Method

$\square$ Now use the $x_{n}$ values already updated on the current iteration to update $x_{k}$

- That is, $x_{n, i+1}$ for $n<k$
$\square$ Gauss-Seidel iterative formula

$$
\begin{equation*}
x_{k, i+1}=\frac{1}{a_{k, k}}\left[y_{k}-\sum_{n=1}^{k-1} a_{k, n} x_{n, i+1}-\sum_{n=k+1}^{N} a_{k, n} x_{n, i}\right], \quad k=1 \ldots N \tag{7}
\end{equation*}
$$

$\square$ Note that only the first summation has changed
$\square$ For already updated $x$ values
$\square x_{n}$ for $n<k$
$\square$ Number of already-updated values used depends on $k$

## Gauss-Seidel - Matrix Form

$\square$ In matrix form the iterative formula is the same as for the Jacobi method

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{M} \mathbf{x}_{i}+\mathbf{D}^{-1} \mathbf{y} \tag{5}
\end{equation*}
$$

where, again

$$
\begin{equation*}
\mathbf{M}=\mathbf{D}^{-1}(\mathbf{D}-\mathbf{A}) \tag{6}
\end{equation*}
$$

but now $\mathbf{D}$ is the lower triangular part of $\mathbf{A}$

$$
\mathbf{D}=\left[\begin{array}{cccc}
a_{1,1} & 0 & \cdots & 0 \\
a_{2,1} & a_{2,2} & 0 & \vdots \\
\vdots & \vdots & \ddots & 0 \\
a_{N, 1} & a_{N, 2} & \cdots & a_{N, N}
\end{array}\right]
$$

$\square$ Otherwise, the algorithm and computer code is identical to that of the Jacobi method

## Gauss-Seidel - Example

$\square$ Apply Gauss-Seidel to our previous example

- $x_{0}=\left[\begin{array}{lll}10 & 25 & 10\end{array}\right]^{T}$

ㅁ $\varepsilon_{s}=1 \times 10^{-6}$

| $\boldsymbol{i}$ | $\mathbf{x}_{\boldsymbol{i}}$ |  | $\boldsymbol{\varepsilon}_{\boldsymbol{i}}$ |
| :---: | :---: | :---: | :---: |
| 0 | $\left[\begin{array}{lll}10 & 25 & 10\end{array}\right]^{T}$ | - |  |
| 1 | $\left[\begin{array}{lll}18.75 & 33.17 & 10.06\end{array}\right]^{T}$ | 0.875 |  |
| 2 | $\left[\begin{array}{lll}18.85 & 33.32 & 10.11\end{array}\right]^{T}$ | 0.005 |  |
| 3 | $\left[\begin{array}{lll}18.94 & 33.47 & 10.16\end{array}\right]^{T}$ | 0.005 |  |
| 4 | $\left[\begin{array}{lll}19.03 & 33.61 & 10.20\end{array}\right]^{T}$ | 0.005 |  |
| $\vdots$ |  | $\vdots$ | $\vdots$ |
| 151 | $\left[\begin{array}{lll}20.50 & 36.00 & 11.00\end{array}\right]^{T}$ | $0.995 \times 10^{-6}$ |  |

$\square$ Convergence achieved in 151 iterations

- Compared to 371 for the Jacobi method


## 65 <br> Nonlinear Systems of Equations

We have seen how to apply the Newton-Raphson rootfinding algorithm to solve a single nonlinear equation. We will now extend that algorithm to the solution of a system of nonlinear equations

## Nonlinear Systems of Equations

$\square$ Consider a system of nonlinear equations

- Can be represented as a vector of $N$ functions
- Each is a function of an $N$-vector of unknown variables

$$
\mathbf{y}=\left[\begin{array}{c}
y_{1} \\
y_{2} \\
\vdots \\
y_{N}
\end{array}\right]=\mathbf{f}(\mathbf{x})=\left[\begin{array}{c}
f_{1}\left(x_{1}, x_{2}, \cdots, x_{N}\right) \\
f_{2}\left(x_{1}, x_{2}, \cdots, x_{N}\right) \\
\vdots \\
f_{N}\left(x_{1}, x_{2}, \cdots, x_{N}\right)
\end{array}\right]
$$

$\square$ As we did when applying Newton-Raphson to find the root of a single equation, we can again approximate this function as linear (i.e., a firstorder Taylor series approximation)

$$
\begin{equation*}
\mathbf{y}=\mathbf{f}(\mathbf{x}) \approx \mathbf{f}\left(\mathbf{x}_{0}\right)+\mathbf{f}^{\prime}\left(\mathbf{x}_{0}\right)\left(\mathbf{x}-\mathbf{x}_{0}\right) \tag{8}
\end{equation*}
$$

- Note that all variables are $N$-vectors
- $\mathbf{f}$ is an $N$-vector of known, nonlinear functions
- $\mathbf{x}$ is an $N$-vector of unknown values - this is what we want to solve for
- $\mathbf{y}$ is an $N$-vector of known values
- $\mathbf{x}_{\mathbf{0}}$ is an $N$-vector of $\mathbf{x}$ values for which $\mathbf{f}\left(\mathbf{x}_{0}\right)$ is known


## Newton-Raphson Method

$\square$ Equation (8) is the basis for our Newton-Raphson iterative formula

- Let it be an equality and solve for $\mathbf{x}$

$$
\begin{aligned}
& \mathbf{y}-\mathbf{f}\left(\mathbf{x}_{0}\right)=\mathbf{f}^{\prime}\left(\mathbf{x}_{0}\right)\left(\mathbf{x}-\mathbf{x}_{0}\right) \\
& {\left[\mathbf{f}^{\prime}\left(\mathbf{x}_{0}\right)\right]^{-\mathbf{1}}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{0}\right)\right]=\mathbf{x}-\mathbf{x}_{0}} \\
& \mathbf{x}=\mathbf{x}_{0}+\left[\mathbf{f}^{\prime}\left(\mathbf{x}_{0}\right)\right]^{\mathbf{- 1}}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{0}\right)\right]
\end{aligned}
$$

$\square$ This last expression can be used as an iterative formula

$$
\mathbf{x}_{i+1}=\mathbf{x}_{i}+\left[\mathbf{f}^{\prime}\left(\mathbf{x}_{i}\right)\right]^{-1}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{i}\right)\right]
$$

$\square$ The derivative term on the right-hand side of (8) is an $N \times N$ matrix

- The Jacobian matrix, J

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{x}_{i}+\mathbf{J}_{i}^{-1}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{i}\right)\right] \tag{9}
\end{equation*}
$$

## The Jacobian Matrix

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{x}_{i}+\mathbf{J}_{i}^{-1}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{i}\right)\right] \tag{9}
\end{equation*}
$$

$\square$ Jacobian matrix

- $N \times N$ matrix of partial derivatives for $\mathbf{f}(\mathbf{x})$
$\square$ Evaluated at the current value of $\mathbf{x}, \mathbf{x}_{i}$

$$
\mathbf{J}_{i}=\left[\begin{array}{cccc}
\frac{\partial f_{1}}{\partial x_{1}} & \frac{\partial f_{1}}{\partial x_{2}} & \cdots & \frac{\partial f_{1}}{\partial x_{N}} \\
\frac{\partial f_{2}}{\partial x_{1}} & \frac{\partial f_{2}}{\partial x_{2}} & \cdots & \frac{\partial f_{2}}{\partial x_{N}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_{N}}{\partial x_{1}} & \frac{\partial f_{N}}{\partial x_{2}} & \cdots & \frac{\partial f_{N}}{\partial x_{N}}
\end{array}\right]_{\mathbf{x}=\mathbf{x}_{i}}
$$

## Newton-Raphson Method

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{x}_{i}+\mathbf{J}_{i}^{-1}\left[\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{i}\right)\right] \tag{9}
\end{equation*}
$$

$\square$ We could iterate (9) until convergence or a maximum number of iterations is reached

- Requires inversion of the Jacobian matrix
- Computationally expensive and error prone
$\square$ Instead, go back to the Taylor series approximation

$$
\begin{align*}
& \mathbf{y}=\mathbf{f}\left(\mathbf{x}_{i}\right)+\mathbf{J}_{i}\left(\mathbf{x}_{i+1}-\mathbf{x}_{i}\right) \\
& \mathbf{y}-\mathbf{f}\left(\mathbf{x}_{i}\right)=\mathbf{J}_{i}\left(\mathbf{x}_{i+1}-\mathbf{x}_{i}\right) \tag{10}
\end{align*}
$$

- Left side of (21) represents a difference between the known and approximated outputs
- Right side represents an increment of the approximation for $\mathbf{x}$

$$
\begin{equation*}
\Delta \mathbf{y}_{i}=\mathbf{J}_{i} \Delta \mathbf{x}_{i} \tag{11}
\end{equation*}
$$

## Newton-Raphson Method

$$
\begin{equation*}
\Delta \mathbf{y}_{i}=\mathbf{J}_{i} \Delta \mathbf{x}_{i} \tag{12}
\end{equation*}
$$

$\square$ On each iteration:
$\square$ Compute $\Delta \mathbf{y}_{i}$ and $\mathbf{J}_{i}$
$\square$ Solve for $\Delta \mathbf{x}_{i}$ using Gaussian elimination

- Matrix inversion not required
- Computationally robust
- Update $\mathbf{x}$

$$
\begin{equation*}
\mathbf{x}_{i+1}=\mathbf{x}_{i}+\Delta \mathbf{x}_{i} \tag{13}
\end{equation*}
$$

## Newton-Raphson - Example

$\square$ Apply Newton-Raphson to solve the following system of nonlinear equations

$$
\begin{aligned}
& \mathbf{f}(\mathbf{x})=\mathbf{y} \\
& {\left[\begin{array}{c}
x_{1}^{2}+3 x_{2} \\
x_{1} x_{2}
\end{array}\right]=\left[\begin{array}{c}
21 \\
12
\end{array}\right]}
\end{aligned}
$$

$\square$ Initial condition: $\mathbf{x}_{0}=\left[\begin{array}{ll}1 & 2\end{array}\right]^{T}$

- Stopping criterion: $\varepsilon_{s}=1 \times 10^{-6}$
- Jacobian matrix

$$
\mathbf{J}_{i}=\left[\begin{array}{ll}
\frac{\partial f_{1}}{\partial x_{1}} & \frac{\partial f_{1}}{\partial x_{2}} \\
\frac{\partial f_{2}}{\partial x_{1}} & \frac{\partial f_{2}}{\partial x_{2}}
\end{array}\right]_{\mathbf{x}=\mathbf{x}_{i}}=\left[\begin{array}{cc}
2 x_{1, i} & 3 \\
x_{2, i} & x_{1, i}
\end{array}\right]
$$

## Newton-Raphson - Example

$$
\begin{align*}
& \Delta \mathbf{y}_{i}=\mathbf{J}_{i} \Delta \mathbf{x}_{i}  \tag{12}\\
& \mathbf{x}_{i+1}=\mathbf{x}_{i}+\Delta \mathbf{x}_{i} \tag{13}
\end{align*}
$$

$\square$ For iteration $i$ :
$\square$ Compute $\Delta \mathbf{y}_{i}$ and $\mathbf{J}_{i}$
$\square$ Solve (12) for $\Delta \mathbf{x}_{i}$
$\square$ Update $\mathbf{x}$ using (13)

## Newton-Raphson - Example

$\square \underline{i=0}:$

$$
\begin{aligned}
& \Delta \mathbf{y}_{0}=\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{0}\right)=\left[\begin{array}{l}
21 \\
12
\end{array}\right]-\left[\begin{array}{l}
7 \\
2
\end{array}\right]=\left[\begin{array}{l}
14 \\
10
\end{array}\right] \\
& \mathbf{J}_{0}=\left[\begin{array}{cc}
2 x_{1,0} & 3 \\
x_{2,0} & x_{1,0}
\end{array}\right]=\left[\begin{array}{ll}
2 & 3 \\
2 & 1
\end{array}\right] \\
& \Delta \mathbf{x}_{0}=\left[\begin{array}{l}
4 \\
2
\end{array}\right] \\
& \mathbf{x}_{1}=\mathbf{x}_{0}+\Delta \mathbf{x}_{0}=\left[\begin{array}{l}
1 \\
2
\end{array}\right]+\left[\begin{array}{l}
4 \\
2
\end{array}\right]=\left[\begin{array}{l}
5 \\
4
\end{array}\right] \\
& \varepsilon_{1}=\max \left(\left|\frac{x_{k, 1}-x_{k, 0}}{x_{k, 1}}\right|\right), \quad k=1 \ldots N \\
& x_{1}=\left[\begin{array}{l}
5 \\
4
\end{array}\right], \quad \varepsilon_{1}=0.8
\end{aligned}
$$

## Newton-Raphson - Example

$\square \underline{i=1}:$

$$
\begin{aligned}
& \Delta \mathbf{y}_{1}=\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{1}\right)=\left[\begin{array}{l}
21 \\
12
\end{array}\right]-\left[\begin{array}{l}
37 \\
20
\end{array}\right]=\left[\begin{array}{c}
-16 \\
-8
\end{array}\right] \\
& \mathbf{J}_{1}=\left[\begin{array}{cc}
2 x_{1,1} & 3 \\
x_{2,1} & x_{1,1}
\end{array}\right]=\left[\begin{array}{cc}
10 & 3 \\
4 & 5
\end{array}\right] \\
& \Delta \mathbf{x}_{1}=\left[\begin{array}{c}
-1.474 \\
-0.421
\end{array}\right] \\
& \mathbf{x}_{2}=\mathbf{x}_{1}+\Delta \mathbf{x}_{1}=\left[\begin{array}{l}
5 \\
4
\end{array}\right]+\left[\begin{array}{c}
-1.474 \\
-0.421
\end{array}\right]=\left[\begin{array}{l}
3.526 \\
3.579
\end{array}\right] \\
& \varepsilon_{2}=\max \left(\left|\frac{x_{k, 2}-x_{k, 1}}{x_{k, 1}}\right|\right), \quad k=1 \ldots N \\
& \quad x_{2}=\left[\begin{array}{c}
3.526 \\
3.579
\end{array}\right], \quad \varepsilon_{2}=0.418
\end{aligned}
$$

## Newton-Raphson - Example

$\square \underline{i=2}:$

$$
\begin{aligned}
& \Delta \mathbf{y}_{2}=\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{2}\right)=\left[\begin{array}{l}
21 \\
12
\end{array}\right]-\left[\begin{array}{l}
23.172 \\
12.621
\end{array}\right]=\left[\begin{array}{l}
-2.172 \\
-0.621
\end{array}\right] \\
& \mathbf{J}_{2}=\left[\begin{array}{cc}
2 x_{1,2} & 3 \\
x_{2,2} & x_{1,2}
\end{array}\right]=\left[\begin{array}{l}
7.053 \\
3.579 \\
3.526
\end{array}\right] \\
& \Delta \mathbf{x}_{2}=\left[\begin{array}{r}
-0.410 \\
0.240
\end{array}\right] \\
& \mathbf{x}_{3}=\mathbf{x}_{2}+\Delta \mathbf{x}_{2}=\left[\begin{array}{l}
3.526 \\
3.579
\end{array}\right]+\left[\begin{array}{r}
-0.410 \\
0.240
\end{array}\right]=\left[\begin{array}{l}
3.116 \\
3.819
\end{array}\right] \\
& \varepsilon_{3}=\max \left(\left|\frac{x_{k, 3}-x_{k, 2}}{x_{k, 2}}\right|\right), \quad k=1 \ldots N \\
& x_{3}=\left[\begin{array}{l}
3.116 \\
3.819
\end{array}\right], \quad \varepsilon_{3}=0.132
\end{aligned}
$$

## Newton-Raphson - Example

$\square \underline{i=6}:$

$$
\begin{aligned}
& \Delta \mathbf{y}_{6}=\mathbf{y}-\mathbf{f}\left(\mathbf{x}_{6}\right)=\left[\begin{array}{l}
21 \\
12
\end{array}\right]-\left[\begin{array}{l}
21.000 \\
12.000
\end{array}\right]=\left[\begin{array}{c}
-0.527 \times 10^{-7} \\
0.926 \times 10^{-7}
\end{array}\right] \\
& \mathbf{J}_{6}=\left[\begin{array}{cc}
2 x_{1,6} & 3 \\
x_{2,6} & x_{1,6}
\end{array}\right]=\left[\begin{array}{l}
6.000 \\
4.000 \\
3.000
\end{array}\right] \\
& \Delta \mathbf{x}_{6}=\left[\begin{array}{c}
-0.073 \times 10^{-6} \\
0.128 \times 10^{-6}
\end{array}\right] \\
& \mathbf{x}_{7}=\mathbf{x}_{6}+\Delta \mathbf{x}_{6}=\left[\begin{array}{l}
3.000 \\
4.000
\end{array}\right]+\left[\begin{array}{r}
-0.073 \times 10^{-6} \\
0.128 \times 10^{-6}
\end{array}\right]=\left[\begin{array}{l}
3.000 \\
4.000
\end{array}\right] \\
& \varepsilon_{7}=\max \left(\left(\left.\frac{x_{k, 7}-x_{k, 6}}{x_{k, 6}} \right\rvert\,\right), \quad k=1 \ldots N\right. \\
& x_{7}=\left[\begin{array}{l}
3.000 \\
4.000
\end{array}\right], \quad \varepsilon_{7}=31.9 \times 10^{-9}
\end{aligned}
$$

## Newton-Raphson - Python Code

$\square$ Define the system of equations

```
f = lambda x: np.array([x[0]**2 + 3*x[1], x[0]*x[1]])
y = np.array([21, 12])
```

$\square$ Initialize x

```
11
12 x0 = np.array([1, 2])
13 x = x0
```

$\square$ Set up solution parameters

```
17
reltol = 1e-6
max_iter = 1000
eps = 1
iter = 0
```


## Newton-Raphson - Python Code

$\square$ Iterate:
Compute $\Delta \mathbf{y}_{i}$ and $\mathbf{J}_{i}$
$\square$ Solve for $\Delta \mathbf{x}_{i}$
$\square$ Update $\mathbf{x}$
25
26
2 7
28
29
30
31
33
34
35
36
37
38

```
```

```
24 while(iter < max_iter) and (eps > reltol):
```

```
24 while(iter < max_iter) and (eps > reltol):
32 # use Gaussian elimination to solve for increment to }
32 # use Gaussian elimination to solve for increment to }
```

J = np.array([[2*x[0], 3], [x[1], x[0]]])

```
J = np.array([[2*x[0], 3], [x[1], x[0]]])
x_old = x
x_old = x
# calculate output error term
# calculate output error term
Dy = y - f(x_old)
Dy = y - f(x_old)
Dx = np.linalg.solve(J, Dy)
Dx = np.linalg.solve(J, Dy)
x = x_old + Dx
x = x_old + Dx
eps = np.max(abs((x - x_old)/x))
eps = np.max(abs((x - x_old)/x))
iter = iter + 1
```

iter = iter + 1

```
```

