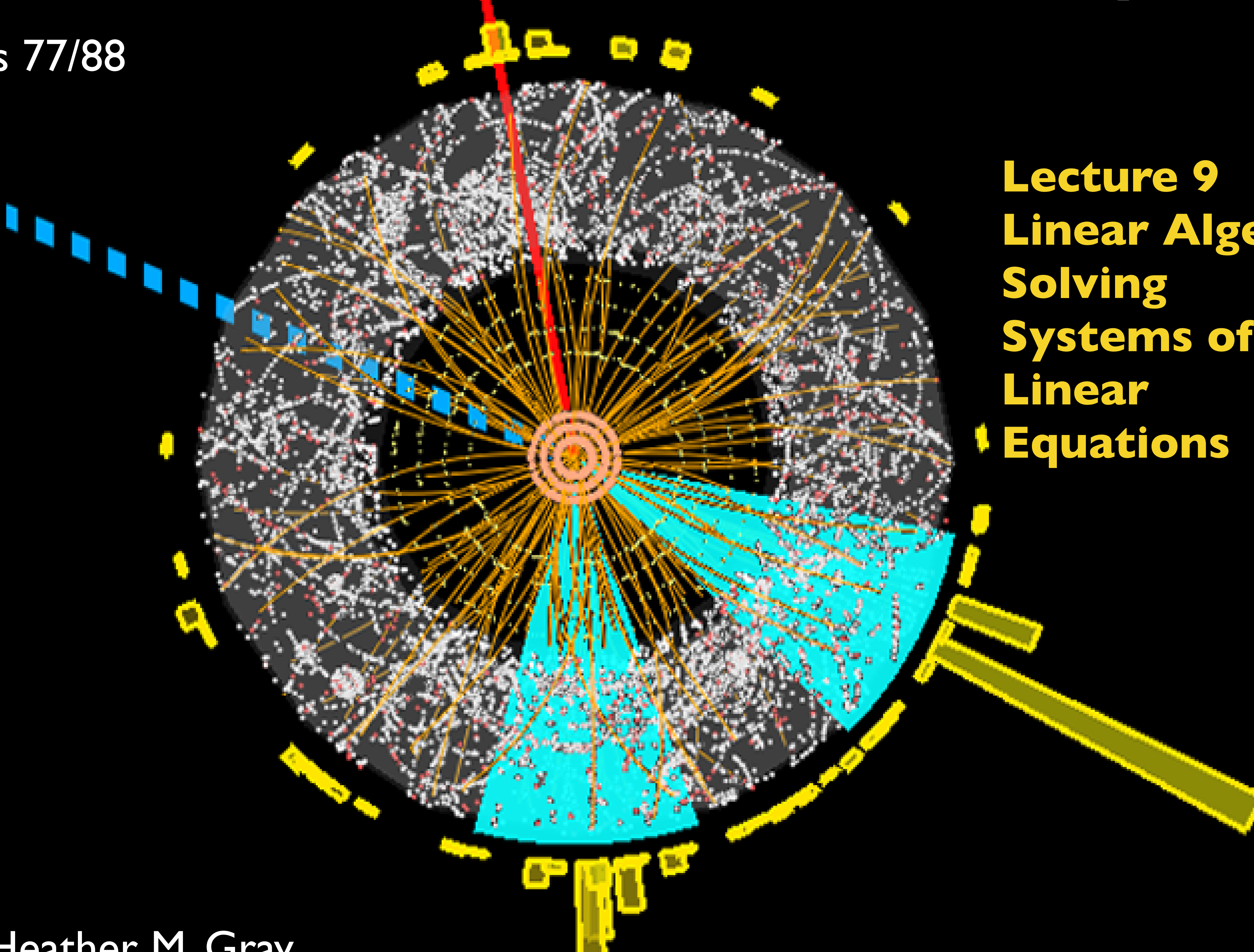
Introduction to Computational Techniques in Physics/Data Science Applications in Physics

Physics 77/88



Lecture 9
Linear Algebra: Solving Systems of Linear Equations

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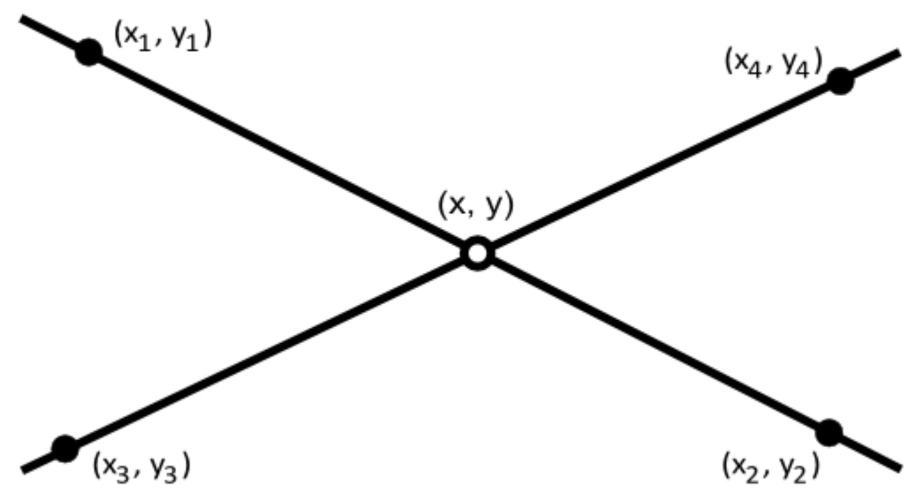
Example: Finding Intersection of Two Lines

- Example 1:
  - $y = 2 - x$
  - $y = x - 1$
- Solution:

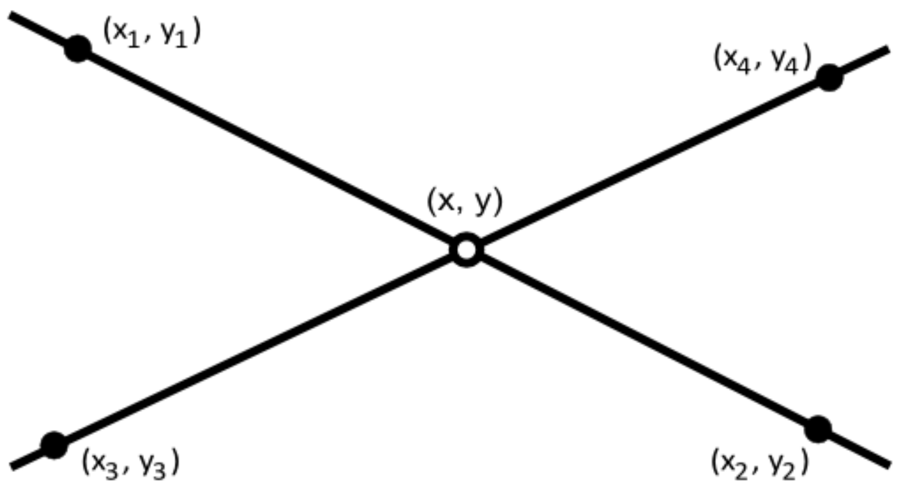


  - $\Rightarrow x =$
  - $y =$
  - $(x, y) =$

$$\begin{bmatrix} & \\ & \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \\ \end{bmatrix}$$

Example: Finding Intersection of Two Lines

- Example 2 (generic):
  - $a_{11}x + a_{12}y = c_1$
  - $a_{21}x + a_{22}y = c_2$
- Solution:



  -

$$\cdot x = \qquad \cdot x \qquad \Rightarrow x = \frac{\quad}{\quad}$$

  -

$$= (\qquad \cdot) x$$

Substitute and solve for y

Linear Algebraic Equations

- $$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots a_{1n}x_n &= c_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots a_{2n}x_n &= c_2 \\ \vdots \quad &= \vdots \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots a_{nn}x_n &= c_n \end{aligned}$$

- $$\begin{bmatrix} & & \cdots & \\ & & \cdots & \\ & & \cdots & \\ \vdots & \vdots & \vdots & \vdots \\ & & \cdots & \end{bmatrix} \begin{Bmatrix} \\ \\ \\ \vdots \\ \\ \end{Bmatrix} = \begin{Bmatrix} \\ \\ \\ \vdots \\ \\ \end{Bmatrix}$$

- In matrix format
    -
- Solution
    -

Linear Algebra Primer: Matrices

- Inverse
  -
- Transpose
  -
- Conjugate transpose
  -
- Trace
  -

Linear Algebra Primer: Matrices

- Symmetric
  -
- Unitary
- Normal
  -

Determinant

- If the of a matrix is then solutions (and)
- Our Generic Example 2:
  - $a_{11}x + a_{12}y = c_1$
  - $a_{21}x + a_{22}y = c_2$
- $x = \dfrac{\dfrac{c_1}{a_{12}} - \dfrac{c_2}{a_{22}}}{\dfrac{a_{11}}{a_{12}} - \dfrac{a_{21}}{a_{22}}}, y = \dfrac{\dfrac{c_2}{a_{21}} - \dfrac{c_1}{a_{11}}}{\dfrac{a_{11}}{a_{12}} - \dfrac{a_{21}}{a_{22}}}$
- If ; x and y are

Determinant of a Matrix

- The determinant is a r that can be used to the matrix
- $\det A = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$
- $= a_{11} \begin{vmatrix} & \\ & \end{vmatrix} - a_{12} \begin{vmatrix} & \\ & \end{vmatrix} + a_{13} \begin{vmatrix} & \\ & \end{vmatrix}$
- =

Aside: Levi-Civita Symbol

- Define $\epsilon_{ij} = \begin{cases} & \text{if } (i,j) = \\ & \text{if } (i,j) = \\ & \text{if} \end{cases}$

- e.g. $\begin{pmatrix} \epsilon_{11} & \epsilon_{12} \\ \epsilon_{21} & \epsilon_{22} \end{pmatrix} = \begin{pmatrix} & \\ & \end{pmatrix}$

- For matrix A $\Rightarrow \det A = \sum$

Aside: Levi-Civita Symbol

- Extending to 3 dimensions

- $$\epsilon_{ijk} = \begin{cases} & \text{if } (i,j,k) = \\ & \text{if } (i,j,k) = \\ & \text{if} \end{cases}$$

- A famous application

- $$a \times b = \left| \quad \right| = \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{k=1}^{3}$$

- $$(a \times b)^i = \sum_{j=1}^{3} \sum_{k=1}^{3}$$

Einstein summation: sum over repeated indices is implied

Aside: Levi-Civita Symbol

- We can generalize to matrices of size
  - $\epsilon_{i_1 i_2 \cdots i_n} = \Bigg\{$
    - if p is the of the from to
      - the number of to get from order to
- Then in n dimensions $A = [a_{ij}]$ and
  - $\det(A) =$

Cramer's Rule

- is the of the with the and removed
- $(-1)^{ij}$ is called the of element a_{ij}
- $\det(A) = \sum_{i=1}^{n}$

Cramer's Rule

$$x_1 = \frac{\left|\qquad\right|}{\left|\qquad\right|} \qquad x_j = \frac{\left|\qquad\right|}{\left|\qquad\right|}$$

Practical Details: Cramer's Rule

- operations for the
- operations for
- for matrix
- error propagation
- for small matrices ($n < 20$)

Gaussian Elimination

- Divide by the
- Subtract from all the
- Move to the and continue

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ a_{31} & a_{32} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix}$$

Gaussian Elimination

- Divide each row by the leading element

$$\begin{bmatrix} \frac{a_{11}}{} & \frac{a_{12}}{} & \cdots & \frac{a_{11}}{} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{a_{31}}{} & \frac{a_{32}}{} & \cdots & \frac{a_{3n}}{} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{a_{n1}}{} & \frac{a_{n2}}{} & \cdots & \frac{a_{nn}}{} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \frac{c_1}{} \\ \vdots \\ \frac{c_3}{} \\ \vdots \\ \frac{c_n}{} \end{bmatrix}$$

Gaussian Elimination

- Subtract row 1 from all the other rows

$$\begin{bmatrix} 1 & \frac{a_{12}}{a_{11}} & \frac{a_{13}}{a_{11}} & \cdots & \frac{a_{11}}{a_{11}} \\ \vdots & \vdots & \vdots & \vdots & \\ 0 & \frac{a_{32}}{a_{31}} - & \frac{a_{33}}{a_{31}} - & \cdots & \frac{a_{3n}}{a_{31}} - \\ \vdots & \vdots & \vdots & \vdots & \\ 0 & \frac{a_{n2}}{a_{n1}} - & \frac{a_{n3}}{a_{n1}} - & \cdots & \frac{a_{nn}}{a_{n1}} - \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \frac{c_1}{a_{11}} \\ \vdots \\ \frac{c_3}{a_{31}} - \\ \vdots \\ \frac{c_n}{a_{n1}} - \end{bmatrix}$$

Gaussian Elimination

$$\begin{bmatrix} 1 & & & \cdots & \\ 0 & 1 & & \cdots & \\ 0 & 0 & 1 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \vdots \\ \\ \end{bmatrix}$$

- Back substitution
  - $x_n =$
  - $x_i =$

Gaussian Elimination: Practical Issues

- Division by
  - May occur in
-
  - Prone to

Gaussian Elimination: Example

- Let's look at the following system of equations
- We're going to use five significant figures with chopping

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

- After forward elimination

$$\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$

Gaussian Elimination: Example

- Next, we apply back substitution

$$\begin{bmatrix} 1 & -.7 & 0 \\ 0 & 1 & -588.23524 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.7 \\ -588.3323 \\ 0.9992235 \end{bmatrix}$$

- $x_3 =$
- $x_2 =$
- $x_1 =$

Gaussian Elimination: Example

- Compare the calculated values with the exact solution
- $$[X]_{\text{exact}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \quad \\ \quad \\ \quad \end{bmatrix}$$
- $$[X]_{\text{calculated}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -0.35 \\ -1.5 \\ 0.99993 \end{bmatrix}$$

Now let’s see how this looks in python

Gaussian Elimination: Improvements

- We can increase the number of
  - Decreases the error
  - Does avoid division
- Gaussian elimination with
  - division by zero
  - rounding off error

Partial Pivoting

- Gaussian elimination with   applies
  to normal Gaussian elimination
- At the beginning of the   of   ,
  find the maximum of
- If the maximum of the values is   in the
  $k \leq p \leq n$
  - Switch
- Gaussian elimination with partial pivoting ensures that
  of forward elimination is performed with the
  having the largest

Example

- Consider the same system of equations
  - $10x_1 - 7x_2 = 7$
  - $-3x_1 + 2.099x_2 + 3x_3 = 3.901$
  - $5x_1 - x_2 + 5x_3 = 6$
- In matrix form
- $\begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$
- Let's solve them using Gaussian elimination with partial pivoting with with

Partial Pivoting: Example

- Forward elimination: step 1
  - Examine the values of the
  - or
- The largest absolute value is 10, which means, following the rules of partial pivoting, we don't switch anything

$$\begin{bmatrix} 10 & 7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

Forward elimination

$$\begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}$$

Partial Pivoting: Example

- Forward elimination, step 2
  - Examine the values of the second column
    - or
  - The largest absolute value is 0.9 so switch row 2 and 3

$$\begin{bmatrix} 1 & -0.7 & 0 \\ 0 & -0.0034 & 2 \\ 0 & -0.9 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.000333 \\ -0.5 \end{bmatrix}$$

Row swap

$$\begin{bmatrix} 1 & -0.7 & 0 \\ & & \\ & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ \\ \end{bmatrix}$$

Partial Pivoting: Example

- Perform forward elimination

$$\begin{bmatrix} 1 & -0.7 & 0 \\ 0 & -0.9 & -1 \\ 0 & -0.0034 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ -0.5 \\ 2.000333 \end{bmatrix}$$

$$\begin{bmatrix} \quad & \quad & \quad \\ \quad & \quad & \quad \\ \quad & \quad & \quad \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \quad \\ \quad \\ \quad \end{bmatrix}$$

Partial Pivoting Example

- Solve the equations through back substitution

$$\begin{bmatrix} 1 & -0.7 & 0 \\ 0 & 1 & 1.1111 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.7 \\ 0.55555 \\ 0.999223 \end{bmatrix}$$

- $x_3 =$
- $x_2 =$
- $x_1 =$

Partial Pivoting: Example

- Compare the and solution
- That they are is a , but it illustrates the of partial pivoting
- $$[X]_{\text{exact}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$
- $$[X]_{\text{calculated}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}$$

Matrix Factorization

- Assume that our matrix **A** can be written as $\mathbf{A} = \mathbf{VU}$ where **V** and **U** are triangular matrices

- $$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} =$$

- $$\begin{bmatrix} & 0 & 0 & \cdots & 0 \\ & & 0 & \cdots & 0 \\ & & & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ & & & \cdots & \end{bmatrix} \begin{bmatrix} & & & \cdots & \\ 0 & & & \cdots & \\ 0 & 0 & & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \end{bmatrix}$$

Matrix Factorization

- We generally look to solve
- Now we can decompose into and , so
- Then we solve for
- And then solve for

Matrix Factorization

- Method: Decompose $[A]$ to $[V]$ and $[U]$

- $$[A] = [V]\,.\,[U] = \begin{bmatrix} 1 & 0 & 0 \\ v_{21} & 1 & 0 \\ v_{31} & v_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- $[U]$ is the same as the at the end of the

- $[V]$ is obtained using the that were used in the

LU Decomposition: Example

- Let's start by finding $[U]$ matrix using the forward elimination procedure of Gaussian elimination
- $$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$
- $$\text{Row2} - \left[\frac{\text{Row1}}{\quad}\right] \times \quad = \begin{bmatrix} \\ 0 & -4.8 & -1.56 \\ \\ \end{bmatrix}$$
- $$\text{Row3} - \left[\frac{\text{Row1}}{\quad}\right] \times \quad = \begin{bmatrix} 25 & 5 & 1 \\ \\ \\ \end{bmatrix}$$

Lower-Upper Decomposition: Example

- Finding the $[U]$ matrix using the forward elimination process of Gaussian elimination

- $$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$

- $$\text{Row3} - \left[\frac{\text{Row2}}{}\right] \times \qquad = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ & & \end{bmatrix}$$

- $$[U] - \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}$$

LU Decomposition: Example

- Finding the $[V]$ matrix using the multipliers used during the forward elimination process
- From the first step of forward elimination
  - $\begin{bmatrix} 1 & 0 & 0 \\ v_{21} & 1 & 0 \\ v_{31} & v_{32} & 1 \end{bmatrix}$
  - $\Rightarrow v_{21} =$
  - $\Rightarrow v_{31} =$

LU Decomposition: Example

- From the second step of forward elimination
- $$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$
- $\Rightarrow v_{32} =$

LU Decomposition: Example

- $$[V] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}$$

- Cross-check: does $[V][U] = [A]$?
-
- $$[V][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} =$$

LU Decomposition: Example

- Now let's use VU factorization to solve the following set of linear equations
- $$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$
- Using the procedure for finding the $[V]$ and $[U]$ matrices
- $$[A] = [V][U] = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}$$

LU Decomposition: Example

- Complete the forward substitution to solve for $[Z] : [L][Z] = [X]$
- $z_1 = 106.8$

  $\Rightarrow z_2 =$

- $=$

  $=$

  $z_3 =$

- $=$

  $=$

- $\Rightarrow [Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$

LU Decomposition: Example

- Now set $[U][X] = [Z]$
  - $$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -.48 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}$$
- Solve for $[X]$
- The three equations become
  -
  -
  -

LU Decomposition: Example

- From the 3rd equation
  - $0.7a_3 = 0.735$

    $\Rightarrow a_3 =$
  - $=$
- Substitute a_3 into the second equation
  - $-4.8a_2 - 1.56a_3 = -96.21$

    $\Rightarrow a_2 =$

    $=$
  - $=$

LU Decomposition: Example

- Substituting a_3 and a_2 using the first equation
  - $25a_1 + 5a_2 + a_3 = 106.8$

    $\Rightarrow a_1 =$

  - $=$

    $=$
- Hence the final solution is
- $\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}$