Lecture 11 (Part 2): Direct Methods for Linear Systems

From the slides of Alessandra Nardi
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Systems of linear equations

- Problem to solve: $A\,x = b$
- Given $A\,x = b$:
  - Is there a solution?
  - Is the solution unique?

Systems of linear equations
Square matrices

- Given Ax = b, where A is square
  - If a solution exists for any b, then the solution for a specific b is unique.

For a solution to exist for any b, the columns of A must span all N-length vectors. Since there are only N columns of the matrix A to span this space, these vectors must be linearly independent.

A square matrix with linearly independent columns is said to be nonsingular.

Methods for solving linear equations

- Direct methods: find the exact solution in a finite number of steps
- Iterative methods: produce a sequence a sequence of approximate solutions hopefully converging to the exact solution

Gaussian Elimination Basics

Gaussian Elimination Method for Solving $A\,x = b$

- A "Direct" Method
  - Finite Termination for exact result (ignoring roundoff)
- Produces accurate results for a broad range of matrices
- Computationally Expensive

Gaussian Elimination Basics

Solve $A\,x = b$

Step 1 A = L U

Step 2 Forward Elimination

Solve $L\,y = b$

Step 3 Backward Substitution

Solve $U\,x = y$

Note: Changing RHS does not imply to recompute LU factorization

Gaussian Elimination Basics

Reminder by 3x3 example

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$\begin{aligned} M_{11}x_1 + M_{12}x_2 + M_{13}x_3 &= b_1 \\ M_{21}x_1 + M_{22}x_2 + M_{23}x_3 &= b_2 \\ M_{31}x_1 + M_{32}x_2 + M_{33}x_3 &= b_3 \end{aligned}$$

Gaussian Elimination Basics

Use Eqn 1 to Eliminate x_1 from Eqn 2 and 3

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$\begin{aligned} M_{11}x_1 + M_{12}x_2 + M_{13}x_3 &= b_1 \\ M_{21}x_1 + M_{22}x_2 + M_{23}x_3 &= b_2 \\ M_{31}x_1 + M_{32}x_2 + M_{33}x_3 &= b_3 \end{aligned}$$

Gaussian Elimination Basics – Key idea

Use Eqn 1 to Eliminate x_1 from Eqn 2 and 3

$$M_{11} x_1 + M_{12} x_2 + M_{13} x_3 = b_1$$

$$\left(M_{22} - \frac{M_{21}}{M_{11}} M_{12} \right) x_2 + \left(M_{23} - \frac{M_{21}}{M_{11}} M_{13} \right) x_3 = b_2 - \frac{M_{21}}{M_{11}} b_1$$

$$\left(M_{32} - \frac{M_{31}}{M_{11}} M_{12} \right) x_2 + \left(M_{33} - \frac{M_{31}}{M_{11}} M_{13} \right) x_3 = b_3 - \frac{M_{31}}{M_{11}} b_1$$

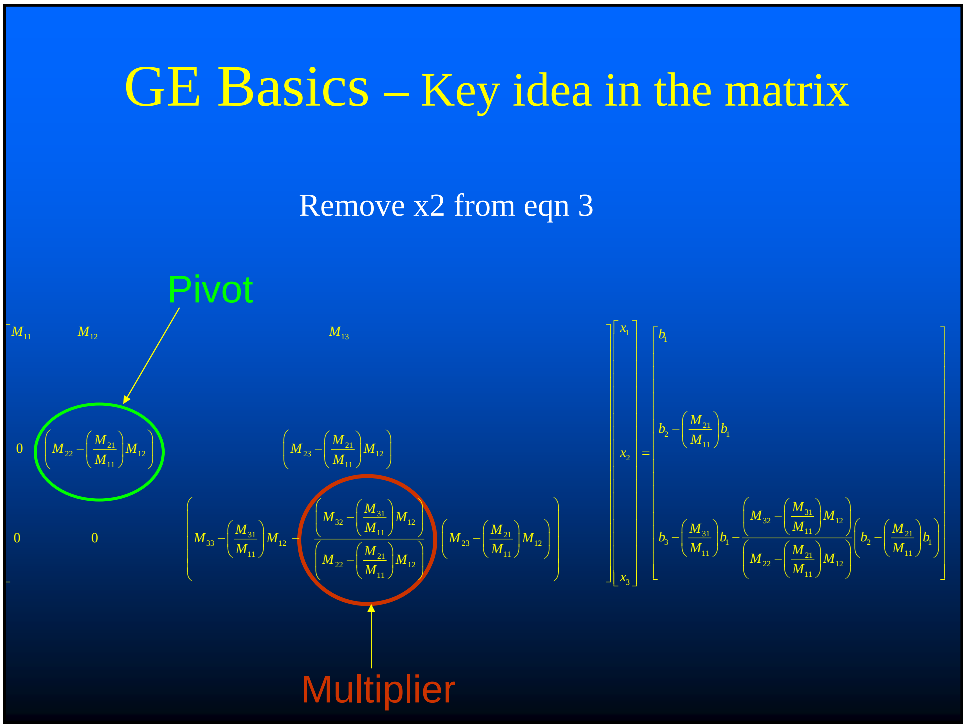
GE Basics – Key idea in the matrix

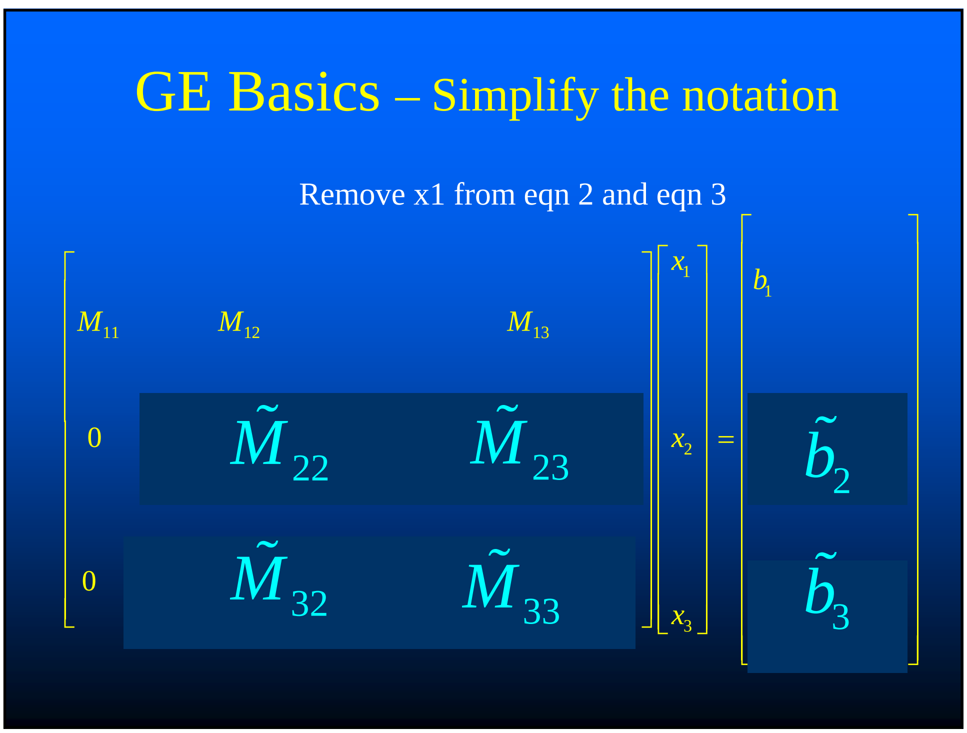
Remove x1 from eqn 2 and eqn 3

Pivot

MULTIPLIERS

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \left(M_{22} - \left(\frac{M_{21}}{M_{11}}\right) M_{12} \right) & \left(M_{23} - \left(\frac{M_{21}}{M_{11}}\right) M_{12} \right) \\ 0 & \left(M_{32} - \left(\frac{M_{31}}{M_{11}}\right) M_{12} \right) & \left(M_{33} - \left(\frac{M_{31}}{M_{11}}\right) M_{12} \right) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 - \left(\frac{M_{21}}{M_{11}}\right) b_1 \\ b_3 - \left(\frac{M_{31}}{M_{11}}\right) b_1 \end{bmatrix}$$


GE Basics – Key idea in the matrix
Remove x2 from eqn 3
Pivot
$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \left(M_{22}-\left(\frac{M_{21}}{M_{11}}\right)M_{12}\right) & \left(M_{23}-\left(\frac{M_{21}}{M_{11}}\right)M_{12}\right) \\ 0 & 0 & \left(M_{33}-\left(\frac{M_{31}}{M_{11}}\right)M_{12}-\frac{\left(M_{32}-\left(\frac{M_{31}}{M_{11}}\right)M_{12}\right)}{\left(M_{22}-\left(\frac{M_{21}}{M_{11}}\right)M_{12}\right)}\left(M_{23}-\left(\frac{M_{21}}{M_{11}}\right)M_{12}\right)\right) \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}=\begin{bmatrix} b_1 \\ b_2-\left(\frac{M_{21}}{M_{11}}\right)b_1 \\ b_3-\left(\frac{M_{31}}{M_{11}}\right)b_1-\frac{\left(M_{32}-\left(\frac{M_{31}}{M_{11}}\right)M_{12}\right)}{\left(M_{22}-\left(\frac{M_{21}}{M_{11}}\right)M_{12}\right)}\left(b_2-\left(\frac{M_{21}}{M_{11}}\right)b_1\right) \end{bmatrix}$$
Multiplier


GE Basics – Simplify the notation
Remove x1 from eqn 2 and eqn 3
$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \tilde{M}_{22} & \tilde{M}_{23} \\ 0 & \tilde{M}_{32} & \tilde{M}_{33} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}=\begin{bmatrix} b_1 \\ \tilde{b}_2 \\ \tilde{b}_3 \end{bmatrix}$$

GE Basics – Simplify the notation

Remove x2 from eqn 3

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \tilde{M}_{22} & \tilde{M}_{23} \\ 0 & 0 & \tilde{M}_{33} - \frac{\tilde{M}_{32}}{\tilde{M}_{22}} \tilde{M}_{23} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ \tilde{b}_2 \\ \tilde{b}_3 - \frac{\tilde{M}_{32}}{\tilde{M}_{22}} \tilde{b}_2 \end{bmatrix}$$

Pivot ($\tilde{M}_{22}$)

Multiplier ($\frac{\tilde{M}_{32}}{\tilde{M}_{22}}$)

GE Basics – GE yields triangular system

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \tilde{M}_{22} & \tilde{M}_{23} \\ 0 & 0 & \tilde{\tilde{M}}_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ \tilde{b}_2 \\ \tilde{\tilde{b}}_3 \end{bmatrix}$$

Altered During GE ($\tilde{b}_2$, $\tilde{\tilde{b}}_3$)

$$\begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

GE Basics – Backward substitution

$$\begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$x_3 = \frac{y_3}{U_{33}}$$

$$x_2 = \frac{y_2 - U_{23} x_3}{U_{22}}$$

$$x_1 = \frac{y_1 - U_{12} x_2 - U_{13} x_3}{U_{11}}$$

GE Basics – RHS updates

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 - \left(\frac{M_{21}}{M_{11}}\right) b_1 \\ b_3 - \left(\frac{M_{31}}{M_{11}}\right) b_1 - \frac{\tilde{M}_{32}}{\tilde{M}_{22}} \tilde{b}_2 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{M_{21}}{M_{11}} & 1 & 0 \\ \frac{M_{31}}{M_{11}} & \frac{\tilde{M}_{32}}{\tilde{M}_{22}} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

GE basics: summary

(1) $A\,x = b$

GE

$U\,x = y$ — Equivalent system

U: upper trg

(2) Noticed that:

$Ly = b$ — *L:* unit lower trg

(3) $U\,x = y$

$LU\,x = b \rightarrow A\,x = b$

$\Rightarrow$ Efficient way of implementing GE: LU factorization

Gaussian Elimination Basics

Solve $A\,x = b$

Step 1 A = L U

Step 2 Forward Elimination

Solve $L\,y = b$

Step 3 Backward Substitution

Solve $U\,x = y$

Note: Changing RHS does not imply to recompute LU factorization

GE Basics – Fitting the pieces together

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{M_{21}}{M_{11}} & 1 & 0 \\ \frac{M_{31}}{M_{11}} & \frac{\tilde{M}_{32}}{\tilde{M}_{22}} & 1 \end{bmatrix}$$

$$U = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \tilde{M}_{22} & \tilde{M}_{23} \\ 0 & 0 & \tilde{\tilde{M}}_{33} \end{bmatrix}$$

GE Basics – Fitting the pieces together

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{M_{21}}{M_{11}} & 1 & 0 \\ \frac{M_{31}}{M_{11}} & \frac{\tilde{M}_{32}}{\tilde{M}_{22}} & 1 \end{bmatrix}$$

$$U = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 0 & \tilde{M}_{22} & \tilde{M}_{23} \\ 0 & 0 & \tilde{\tilde{M}}_{33} \end{bmatrix}$$

$$\begin{bmatrix} M_{11} & M_{21} & M_{31} \\ \frac{M_{21}}{M_{11}} & \tilde{M}_{22} & \tilde{M}_{23} \\ \frac{M_{31}}{M_{11}} & \frac{\tilde{M}_{32}}{\tilde{M}_{22}} & \tilde{\tilde{M}}_{33} \end{bmatrix}$$

LU Basics – Computational Complexity

For i = 1 to n-1 { "For each Row"

For j = i+1 to n { "For each target Row below the source"

$$M_{ji} = \frac{M_{ji}}{M_{ii}}$$ Pivot

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

For k = i+1 to n { "For each Row element beyond Pivot"

$$M_{jk} \leftarrow M_{jk} - M_{ji} M_{ik}$$

Multiplier

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

Multiply-adds

}

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LU Basics – Limitations of the naïve approach

- Zero Pivots

Consider $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

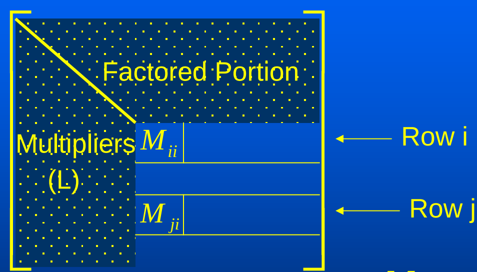
- What about small Pivots (Round-off error)

Consider $\begin{pmatrix} 10^{-15} & 1 \\ 1 & 0 \end{pmatrix}$

$\Rightarrow$ both can be solved with partial pivoting

LU Basics – Partial pivoting for zero pivots

At Step i



What if $M_{ii} = 0$? Cannot form $\frac{M_{ji}}{M_{ii}}$

Simple Fix (Partial Pivoting)

If $M_{ii} = 0$

Find $M_{ji} \neq 0 \quad j > i$

Swap Row j with i

LU Basics – Partial pivoting for zero pivots

Two Important Theorems

1) Partial pivoting (swapping rows) always* succeeds if M is non singular

2) LU factorization applied to a diagonally dominant matrix will never produce a zero pivot

LU Basics – Partial pivoting for small pivots

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 12.5 & 12.5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ 75 \end{bmatrix}$$

GE

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 0 & 12.5 - 1.25\cdot 10^{5} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ 75 - 6.25\cdot 10^{5} \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{5digits} = \begin{bmatrix} 1.0001 \\ 4.9999 \end{bmatrix}$$

LU Basics – Partial pivoting for small pivots

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 12.5 & 12.5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ 75 \end{bmatrix}$$

GE

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 0 & 12.5 - 1.25\cdot 10^{5} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ 75 - 6.25\cdot 10^{5} \end{bmatrix}$$

Rounded to 3 digits

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 0 & -1.25\cdot 10^{5} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ -6.25\cdot 10^{5} \end{bmatrix}$$

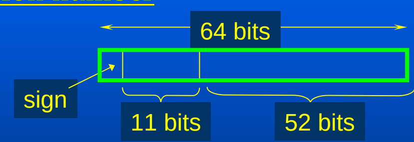
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{3digits} = \begin{bmatrix} 0 \\ 5 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{5digits} = \begin{bmatrix} 1.0001 \\ 4.9999 \end{bmatrix}$$

LU Basics – Partial pivoting for small pivots

An Aside on Floating Point Arithmetic

Double precision number



Basic Problem

Avoid sum and subtraction of large and tiny numbers

$\Rightarrow$ Avoid big multipliers

LU Basics – Partial pivoting for small pivots

Partial Pivoting for Roundoff reduction

$$\text{If } |M_{ii}| < \max_{j>i} |M_{ji}|$$

$$\text{Swap row } i \text{ with } \arg(\max_{j>i} |M_{ij}|)$$

Small Multipliers

LU Basics – Partial pivoting for small pivots

swap

$$\begin{bmatrix} 1.25\cdot 10^{-4} & 1.25 \\ 12.5 & 12.5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6.25 \\ 75 \end{bmatrix}$$

$$\begin{bmatrix} 12.5 & 12.5 \\ 1.25\cdot 10^{-4} & 1.25 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 75 \\ 6.25 \end{bmatrix}$$

GE

$$\begin{bmatrix} 12.5 & 12.5 \\ 0 & 1.25 - 12.5\cdot 10^{-5} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 75 \\ 6.25 - 75\cdot 10^{-5} \end{bmatrix}$$

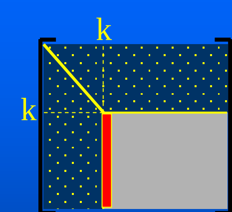
Rounded to 3 digits

$$\begin{bmatrix} 12.5 & 12.5 \\ 0 & 1.25 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 75 \\ 6.25 \end{bmatrix}$$

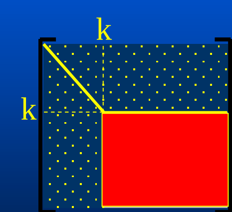
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{3digits} = \begin{bmatrix} 1 \\ 5 \end{bmatrix} \qquad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{5digits} = \begin{bmatrix} 1.0001 \\ 4.9999 \end{bmatrix}$$

Pivoting strategies

- Partial Pivoting:
  - Only row interchange



- Complete Pivoting
  - Row and Column interchange



- Threshold Pivoting
  - Only if prospective pivot is found to be smaller than a certain threshold

Summary

- Existence and uniqueness review
- Gaussian elimination basics
  - GE basics
  - LU factorization
  - Pivoting