Computational Methods
CMSC/AMSC/MAPL 460

Vectors, Matrices, Linear Systems, LU Decomposition,

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Gaussian Elimination

- Zero elements of first column below 1st row
  - multiplying 1st row by 0.3 and add to 2nd row
  - multiplying 1st row by -0.5 and add to 3rd row
  - Results in
- Zero elements of first column below 2nd row
  - Swap rows
  - Multiply 2nd row by 0.04 and add to 3rd

$$\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 4 \\ 6 \end{pmatrix}$$

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -0.1 & 6 \\ 0 & 2.5 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 6.1 \\ 2.5 \end{pmatrix}$$

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.1 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 2.5 \\ 6.1 \end{pmatrix}$$

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 2.5 \\ 6.2 \end{pmatrix}$$

Pivoting

- Every step involves dividing by diagonal in the current row
- Algorithm – should work for general data
- Remember: whenever an algorithm calls for division, we need to check if the entry being divided by can become zero (or almost zero).
- Consider
- Here the system has solution
- Yet division by zero would occur!
- Fix: rearrange the system
- Element by which we divide is called "Pivot element"
- Changing the pivot element is called "pivoting"
- Partial Pivoting and Full Pivoting

$$\begin{bmatrix} 0 & 4 & 4 \\ 4 & 0 & 2 \\ 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \\ 0 \end{bmatrix}$$

$$x = [1, 2, -1]^T$$

Partial Pivoting

- Interchange rows below the current row to ensure that the largest element by magnitude is in the current row
- Also possible to do column interchanges in addition to row interchanges (called full pivoting)

Solution

- Start from last equation which can be solved by division
- Next substitute in the previous line and continue
- This describes the way to do the algorithm by hand
- How to represent it using matrices?
- Also, how do we solve another system that has the same matrix?
  - Upper triangular matrix we end up with will be the same, but the sequence of operations on the r.h.s needs to be repeated

$$6.2x_3 = 6.2$$

$$2.5x_2 + (5)(1) = 2.5.$$

$$10x_1 + (-7)(-1) = 7$$

$$x = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}$$

Gaussian Elimination: LU Matrix decomposition

- It turns out that Gaussian elimination corresponds to a particular matrix decomposition …
  - Product of permutation, lower triangular and upper triangular matrices
- What is a permutation matrix?
  - It rearranges a system of equations and changes the order.
  - Multiplying by it swaps the order of rows in a matrix
  - Essentially a rearrangement of the identity
  - Nice property: transpose is its inverse: $PP^T=I$

$$P = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$Px = b$$

$$x = P^T b$$

- Book keeping to account for changes in a permutation matrix
- (If we did full pivoting we need two permutation matrices to account in addition for column interchanges)

LU Decomposition

- What is an upper triangular matrix?
  - Elements below diagonal are zero

$$U = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 0 & 5 & 6 & 7 \\ 0 & 0 & 8 & 9 \\ 0 & 0 & 0 & 10 \end{pmatrix}$$

- Lower triangular matrix
- Elements above diagonal are zero
- Unit lower triangular matrix
- Elements along diagonal are one

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 3 & 5 & 1 & 0 \\ 4 & 6 & 7 & 1 \end{pmatrix}$$

- Upper triangular part of Gauss Elimination is clear …
  - final matrix we end up with
- What about lower triangular and permutation?

$LU{=}PA$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ -0.3 & -0.04 & 1 \end{pmatrix} \quad U = \begin{pmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.2 \end{pmatrix} \quad P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

- Identify the elements of L and P?
- L has the multipliers we used in the elimination steps
- P has a record of the row swaps we did to avoid dividing by small numbers
- In fact we can write each step of Gaussian elimination in matrix form

$$\begin{aligned} U &= M_{n-1}P_{n-1}\cdots M_2P_2M_1P_1A \\ L_1L_2\cdots L_{n-1}U &= P_{n-1}\cdots P_2P_1A \end{aligned}$$

$$A = \begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} \qquad \begin{aligned} L &= L_1 L_2 \cdots L_{n-1} \\ P &= P_{n-1} \cdots P_2 P_1 \end{aligned}$$

the matrices defined during the elimination are

$$P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0.3 & 1 & 0 \\ -0.5 & 0 & 1 \end{pmatrix},$$

$$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \; M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0.04 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix}$$

$$P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0.3 & 1 & 0 \\ -0.5 & 0 & 1 \end{pmatrix},$$

$$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \; M_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0.04 & 1 \end{pmatrix},$$

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ -0.3 & 0 & 1 \end{pmatrix}, \; L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.04 & 1 \end{pmatrix},$$

Solving a system with the LU decomposition

$Ax=b$

$LU=PA$

$P^T LUx=b$

$L[Ux]=Pb$

Solve $Ly=Pb$

Then $Ux=y$

How good are the answers given by LU?

- In general we cannot determine the exact answer.
- Rather we will determine answer (possibly incorrect), and use it to find how poorly it does in predicting the right hand side
- Difference in r.h.s is the "residual" and is a measure of the error

$$\begin{aligned} r &\equiv b - Ax \\ &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 & 1 \\ \delta & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 0 \\ \delta \end{bmatrix}. \end{aligned}$$

Suppose $\delta < .5 * \epsilon_{mach}$.

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

; system without pivoting, we'll get

$$\begin{bmatrix} \delta & 1 \\ 0 & -1/\delta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -1/\delta \end{bmatrix}$$

$$x_2 = 1, \quad x_1 = 0.$$

True solution

$$x = \begin{bmatrix} -\frac{1}{1-\delta} \\ \frac{1}{1-\delta} \end{bmatrix}$$

With pivoting we get

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

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

$$x_2 = 1, \quad x_1 = -1.$$

- Recall “backward error analysis”
- Determine region in “problem space” where the problem we solved lies
- Here the problem we solved is $Ax=b-r$
- Theorem
  - Gauss elimination with partial pivoting produces small residuals
- Next question:
  - Does a small residue mean a small forward error?
  - Here it did

Example 2

- Compute via GE with partial pivoting

Let's assume 3-digit decimal arithmetic.

$$\begin{bmatrix} .780 & .563 \\ .913 & .659 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} .217 \\ .254 \end{bmatrix}$$

If we compute the solution with pivoting, we obtain

$$x = \begin{bmatrix} -.443 \\ 1.000 \end{bmatrix}, \quad r = \begin{bmatrix} -.000460 \\ -.000541 \end{bmatrix}$$

- However true solution is $[1.000 \quad -1.000]^t$
- Residual was small, but error is large!
- Why?
- Recall condition number

Condition Number of a Matrix

A measure of how close a matrix is to singular

$$\text{cond}(A) = \kappa(A) = \|A\| \cdot \|A^{-1}\|$$

$$= \frac{\text{maximum stretch}}{\text{maximum shrink}} = \frac{\max_i |\lambda_i|}{\min_i |\lambda_i|}$$

- cond(I) = 1
- cond(singular matrix) = ∞
- So even though residual was small, error was multiplied by the condition number, and was significant