CS 357: Numerical Methods

Lecture 7: LU with Pivoting

Eric Shaffer

Elimination Matrices

- Annihilate entries below k^{th} element in a by a transformation:

$$M_k a = \begin{bmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & 0 & \dots & 0 \\ 0 & \dots & -m_{k+1} & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & -m_n & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

  where $m_i = a_i / a_k$, $i = k+1, \dots, n$.
- The divisor a_k is the "pivot" (and needs to be nonzero)

Elimination Matrices

- Matrix M_k is an "elementary elimination matrix": adds a multiple of row k to each subsequent row, with "multipliers" m_i so that the result is zero in the k^{th} column for rows $i > k$.
- M_k is unit lower triangular and nonsingular
- $M_k = I - m_k e_k^T$ where $m_k = [0, \ldots, 0, m_{k+1}, \ldots, m_n]^T$ and e_k is the k^{th} column of the identity matrix I.
- $M_k^{-1} = I + m_k e_k^T$, which means M_k^{-1} is also lower triangular, and we will denote $M_k^{-1} = L_k$.

Can you prove $M_k^{-1} = I + m_k e_k^T$?

Example

Let $a = \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix}$.

$$M_1 a = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

and

$$M_2 a = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$

Example

So

$$L_1 = M_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix},\; L_2 = M_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/2 & 1 \end{bmatrix}$$

which means

$$M_1 M_2 = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 1/2 & 1 \end{bmatrix},\; L_1 L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1/2 & 1 \end{bmatrix}$$

Gaussian Elimination with Elementary Elimination Matrices

- To reduce $Ax = b$ to upper triangular form, first construct M_1 with a_{11} as the pivot (eliminating the first column of A below the diagonal.
- Then $M_1Ax = M_1b$ still has the same solution.
- Next construct M_2 with pivot a_{22} to eliminate the second column below the diagonal.
- Then $M_2M_1Ax = M_2M_1b$ still has the same solution
- $M_{n-1} \dots M_1Ax = M_{n-1} \dots M_1b$
- Let $M = M_nM_{n-1} \dots M_1$; then $MAx = Mb$, with MA upper triangular. Then back solve.

Another Way to Look at A

We've mentioned L and U today. Why?
Consider this

$$A = A$$
$$A = (M^{-1}M)A$$
$$A = (M_1^{-1}M_2^{-1}\ldots M_n^{-1})(M_nM_{n-1}\ldots M_1)A$$
$$A = (M_1^{-1}M_2^{-1}\ldots M_n^{-1})((M_nM_{n-1}\ldots M_1)A)$$

But MA is upper triangular, and we've seen that $M_1^{-1}\ldots M_n^{-1}$ is lower triangular. Thus, we have an algorithm that factors A into two matrices L and U.

Quick Aside: Singular Matrices

- Is the matrix singular? $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

  yes

- Does it have an LU decomposition?

  Yes

  $\underbrace{\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}}_{U}$

Need for pivoting (the obvious case)

- Is this matrix singular?

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

NO

- Does it have an LU decomposition?

Not unless we use pivoting to swap rows

Need for pivoting (the less obvious case)

- Small pivots are bad

$$\begin{bmatrix} e & 1 \\ 1 & 1 \end{bmatrix},$$

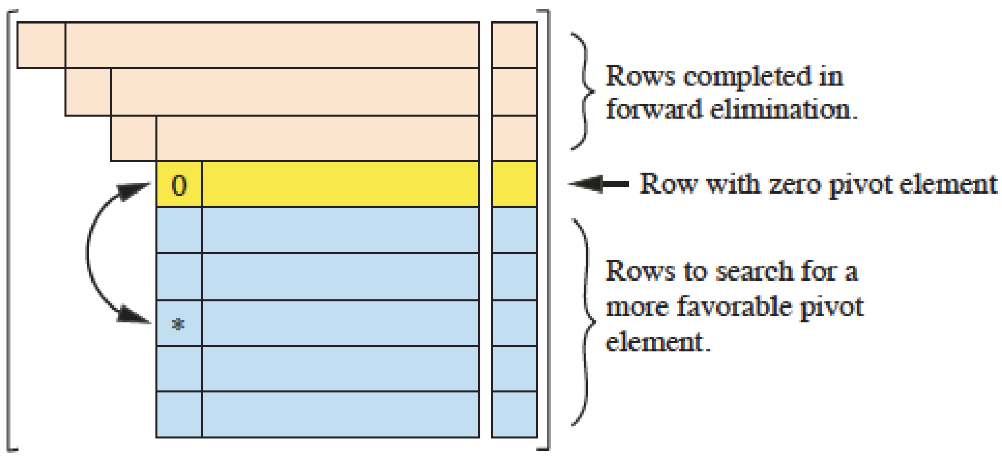
- We'll discuss why when we talk about floating point

- Solution exchange rows so that the largest entry on or below the diagonal becomes the pivot.
- Why on or below?

Partial Pivoting

To avoid division by zero, swap the row having the zero pivot with one of the rows below it.

Partial Pivoting → row swaps



Full Pivoting → row + column

To minimize the effect of roundoff, always choose the row that puts the largest pivot element on the diagonal, i.e., find i_p such that $|a_{i_p,i}| = \max(|a_{k,i}|)$ for $k = i, \ldots, n$

Permutation Matrices

- P is a permutation matrix
  - it is a row-wise reordering of the identity matrix.
  - PA will reorder the rows of A
- Example $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Permutation Matrices

- Example $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \begin{bmatrix} d & e & f \\ a & b & c \\ g & h & i \end{bmatrix}$

Permutation Matrices: Inverse

- Example $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$

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

$$= I$$

Partial Pivoting - Example

$$\begin{bmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{bmatrix} \begin{bmatrix} x1 \\ x2 \\ x3 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \\ 10 \end{bmatrix}$$

$$P_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$M_1 P_1 A x = \begin{bmatrix} 4 & 4 & 2 \\ 0 & 1 & 1.5 \\ 0 & 2 & 2 \end{bmatrix} x$$

$$M_1 = \begin{bmatrix} 1 & 0 & 0 \\ -0.25 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$M_1 P_1 b = \begin{bmatrix} 6 \\ 1.5 \\ 4 \end{bmatrix}$$

Partial Pivoting - Example

$$P_2 = \begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$$

$$M_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.5 & 1 \end{bmatrix}$$

$$M_2 P_2 M_1 P_1 A = \begin{bmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{bmatrix} \quad x = \begin{bmatrix} 6 \\ 4 \\ -0.5 \end{bmatrix}$$

Partial Pivoting - Example

$$\text{"}L\text{"} = M^{-1} = (M_2 P_2 M_1 P_1)^{-1}$$

$$= P_1^T L_1 P_2^T L_2$$

$$= \begin{bmatrix} 0.25 & 0.5 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix}$$

$$P_2 P_1 \text{"}L\text{"} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0.25 & 0.5 & 1 \end{bmatrix}$$

Partial Pivoting - Example

$$PA = LU$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0.75 & 0.5 & 1 \end{bmatrix} \begin{bmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{bmatrix}$$

Partial Pivoting - Example

Partial Pivoting - Example

When do you not need to pivot?

- *Diagonally dominant* matrices where

$$\sum_{i=1, i \neq j}^{n} |a_{ij}| < |a_{jj}|$$

When do you not need to pivot?

- Symmetric Positive Definite Matrices
  - $A = A^T$
  - $x^T A x > 0$ for all $x \neq 0$
- Cholesky Factorization is an option
  - $A = LL^T$
  - No pivoting
  - Only need to store lower triangle of A
  - Half as much work as LU factorization

Aside: Computational Complexity of Matrix Multiplication

$$\underset{n\times n}{A}\ \underset{n\times n}{B} = \underset{n\times n}{C}$$

n^2 entries in C

each a dot product of 2 n vectors:

$$\underbrace{a_1b_1 + \dots + a_nb_n}_{O(n)\text{ operations}}$$

$$\boxed{O(n^3)}$$

Aside: Don’t Use Cramer’s Rule

$$x_i = \frac{\det(A_i)}{\det(A)} \qquad i = 1, \ldots, n$$

2x2 det require 3 operations
3x3 require 3 2x2 determinants plus 5 more operations

So, in general:
Wn> n(Wn-1) > n(n-1)(Wn-2)…>n!

Aside: Don't Use Cramer's Rule

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So, in general:
Wn> n(Wn-1) > n(n-1)(Wn-2)…>n!

20x20 system requires around 2.4×10^{18} operations
At 10^9 flops, that takes 76 years

Solving Banded Systems

A tridiagonal matrix A

$$\begin{bmatrix} d_1 & c_1 & & & & & & \\ a_1 & d_2 & c_2 & & & & & \\ & a_2 & d_3 & c_3 & & & & \\ & & \cdots & \cdots & \cdots & & & \\ & & & a_{i-1} & d_i & c_i & & \\ & & & & \cdots & \cdots & \cdots & \\ & & & & \cdots & \cdots & \cdots & \\ & & & & & & a_{n-1} & d_n \end{bmatrix}$$

- storage is saved by not saving zeros
- only $n+2(n-1)=3n-2$ places are needed to store the matrix versus n^2 for the whole system
- can operations be saved? yes!

Tridiagonal Systems

$$\begin{bmatrix} d_1 & c_1 & & & & & & \\ a_1 & d_2 & c_2 & & & & & \\ & a_2 & d_3 & c_3 & & & & \\ & & \dots & \dots & \dots & & & \\ & & & a_{i-1} & d_i & c_i & & \\ & & & & \dots & \dots & \dots & \\ & & & & \dots & \dots & \dots & \\ & & & & & & a_{n-1} & d_n \end{bmatrix}$$

Start forward elimination (without any special pivoting)

1. subtract a_1/d_1 times row 1 from row 2
2. this eliminates a_1, changes d_2 and does not touch c_2
3. continuing:

$$d_i = d_i - \left(\frac{a_{i-1}}{d_{i-1}} c_{i-1}\right)$$

for $i = 2 \dots n$

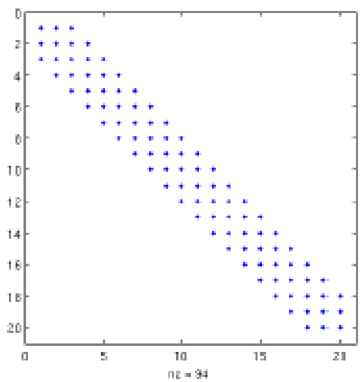
Tridiagonal Systems

$$\begin{bmatrix} \tilde{d}_1 & c_1 & & & & & & \\ & \tilde{d}_2 & c_2 & & & & & \\ & & \tilde{d}_3 & c_3 & & & & \\ & & & \cdots & \cdots & & & \\ & & & & \tilde{d}_i & c_i & & \\ & & & & & \cdots & \cdots & \\ & & & & & \cdots & \cdots & \\ & & & & & & & \tilde{d}_n \end{bmatrix}$$

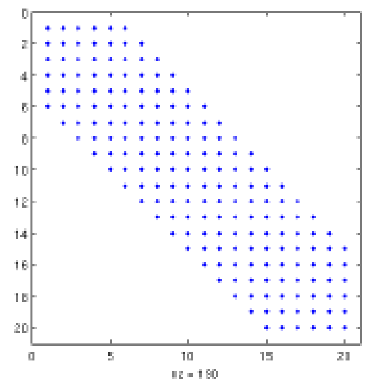
This leaves an upper triangular (2-band). With back substitution:

1. $x_n = \tilde{b}_n / \tilde{d}_n$
2. $x_{n-1} = (1/\tilde{d}_{n-1})(\tilde{b}_{n-1} - c_{n-1} x_n)$
3. $x_i = (1/\tilde{d}_i)(\tilde{b}_i - c_i x_{i+1})$

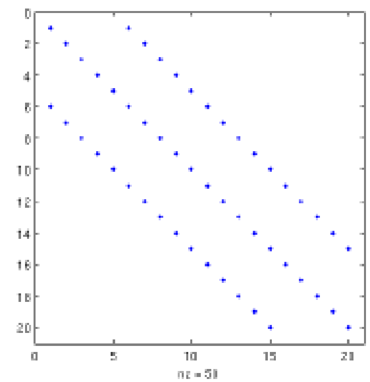
M-Band Systems



$m = 5$



$m = 11$



$m = 11$

- the m correspond to the total width of the non-zeros
- after a few passes of GE *fill-in* with occur within the band
- so an empty band costs (about) the same an a non-empty band
- one fix: reordering (e.g. Cuthill-McKee)
- generally GE will cost $\mathcal{O}(m^2 n)$ for m-band systems