CS 357: Numerical Methods

Lecture 7: LU with Pivoting

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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
- $M_{n-1} \ldots M_1Ax = M_{n-1} \ldots M_1b$
- Let $M = M_nM_{n-1} \ldots M_1$; 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

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

But MA is upper triangular, and we've seen that $M_1^{-1}\dots M_n^{-1}$ 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?

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

- Does it have an LU decomposition?

Need for pivoting (the obvious case)

- Is this matrix singular?

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

- Does it have an LU decomposition?

Need for pivoting (the less obvious case)

- Small pivots are bad

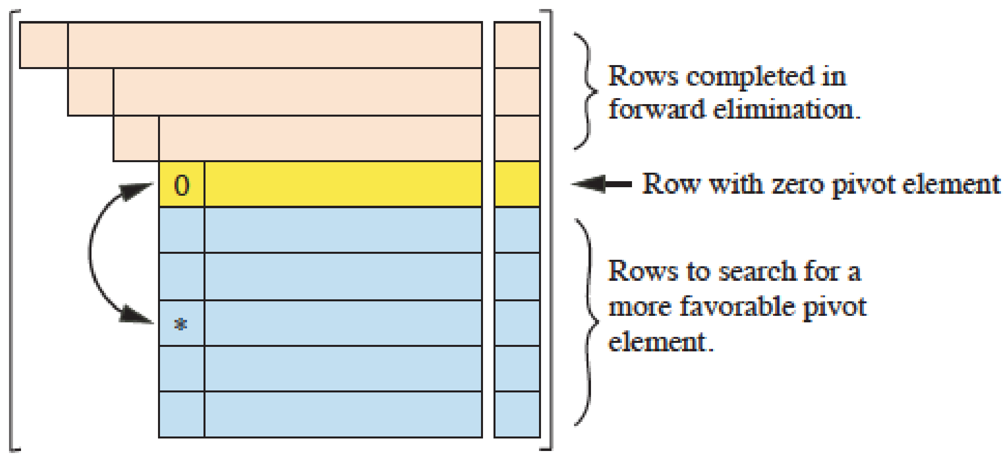
$$\begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix}$$

- 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.



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

Partial Pivoting - Example

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

Partial Pivoting - Example

Partial Pivoting - Example

Partial Pivoting - Example

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

Aside: Don’t Use Cramer’s Rule

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 $i = 2 \dots n$

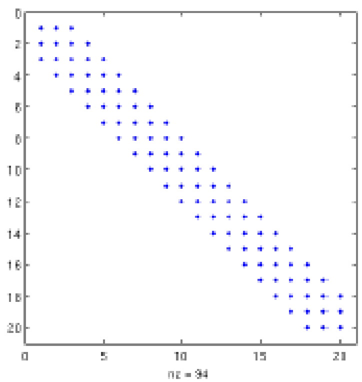
Tridiagonal Systems

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

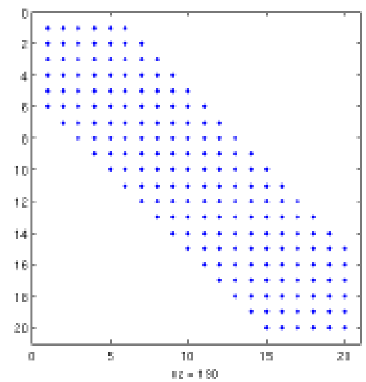
This leaves an upper triangular (2-band). With back substitution:

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. $x_i = (1/\tilde{d}_i)(\tilde{b}_i - c_i x_{i+1})$

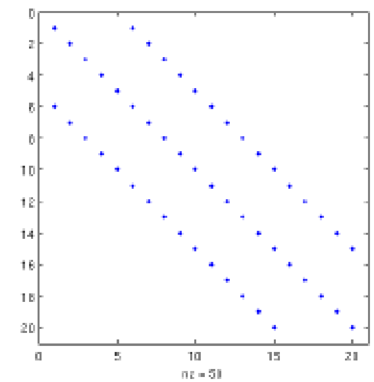
M-Band Systems



$m = 5$



$m = 11$



$m = 11$

- 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