CS412: Lecture #17

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Solving linear systems of equations

Consider a lower triangular matrix L:

| | l_{11} | 0 | 0 | | 0 |
|-----|----------|--------------------|----------|-------|----------|
| | l_{21} | l_{22} | 0 | | 0 |
| L = | l_{31} | $l_{22} \\ l_{32}$ | l_{33} | | 0 |
| - | : | | | | : |
| | l_{n1} | | | | l_{nn} |
| | "n1 | ••• | ••• | • • • | "nn |

A procedure similar to that for upper triangular systems can be followed to solve Lx = b. The overall complexity is again $O(n^2)$.

Algorithm 1 Forward substitution for Lx = b:

| - | | | | |
|---|-------------------------------------|--|--|--|
| 1: for $j = 1n$ do | | | | |
| 2: if $l_{jj} = 0$ then | | | | |
| 3: return. | \triangleright matrix is singular | | | |
| 4: end if | | | | |
| 5: $x_j \leftarrow b_j / l_{jj}$ | | | | |
| 6: for $i = j + 1 \dots n$ do | | | | |
| 7: $b_i \leftarrow b_i - l_{ij} x_j$ | | | | |
| 8: end for | | | | |
| 9: end for | | | | |

The forward and backward substitution processes can be used to solve a non-triangular system by virtue of the following factorization property.

Theorem 1. If A is an $n \times n$ matrix, it can be (generally) written as a product:

A = LU

where L is a lower triangular matrix and U is an upper triangular matrix. Furthermore, it is possible to construct L such that all diagonal elements $l_{ii} = 1$.

Algorithm 2 LU factorization by Gaussian Elimination

1: for k = 1 ... n - 1 do if $a_{kk} = 0$ then 2: return. 3: end if 4:for $i = k + 1 \dots n$ do 5: $a_{ik} \leftarrow a_{ik}/a_{kk}$ 6: end for 7: for $j = k + 1 \dots n$ do 8: for $i = k + 1 \dots n$ do 9: $a_{ij} \leftarrow a_{ij} - a_{ik}a_{kj}$ 10:end for 11:end for 12:13: end for

Note that this algorithm executes in-place, i.e., the matrix A is *replaced* by its LU factorization, in compact form. More specifically, this algorithm produces a factorization A = LU, where:

$$L = \begin{bmatrix} 1 & & & & \\ l_{21} & 1 & & & O \\ l_{31} & l_{32} & 1 & & & \\ l_{41} & l_{42} & l_{43} & 1 & & \\ \vdots & \vdots & \vdots & \ddots & \\ l_{n1} & n_{n2} & l_{n3} & \dots & l_{n,n-1} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \dots & u_{1n} \\ u_{22} & u_{23} & \dots & u_{2n} \\ u_{33} & \dots & u_{3n} \\ O & & \ddots & u_{n-1,n} \\ u_{nn} \end{bmatrix}$$

After the in-place factorization algorithm completes, A is replaced by the following "compacted" encoding of L and U together:

$$A = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \dots & u_{1n} \\ l_{21} & u_{22} & u_{23} & \dots & u_{2n} \\ l_{31} & l_{32} & u_{33} & \dots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \dots & l_{n-1,n} & u_{nn} \end{bmatrix}$$

Here is a slightly different algorithm for Gaussian Elimination via *elimination* matrices. Define the basis vector e_k as:

$$e_k = \left(\begin{array}{c} 0\\ \vdots\\ 0\\ 1\\ 0\\ \vdots\\ 0 \end{array} \right)$$

where the 1 is in the kth row and the length of e_k is n. In order to perform Gaussian Elimination on the kth column a_k of A, we define the $n \times n$ elimination matrix $M_k = I - m_k e_k^T$ where

$$m_k = \frac{1}{a_{kk}} \cdot \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{k+1,k} \\ \vdots \\ a_{n,k} \end{pmatrix}$$

 M_k adds multiples of row k to the rows >k in order to create 0's. As an example, for $a_k=(2,4,-2)^T$

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

Similarly,

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

The inverse of an elimination matrix is defined as $L_k = M_k^{-1} = I + m_k e_k^T$. For example,

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

The algorithm now proceeds as follows. Consider the example:

$$\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix}$$

First, we eliminate the lower triangular portion of A one column at a time using M_k to get $U = M_{n-1} \dots M_1 A$. Note that we also carry out the operations on b to get a new system of equations $M - 2M_1Ax = M_2M_1b$ or $Ux = M_2M_1b$ which can be solved for via back substitution.

$$M_1 A = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix}$$

$$M_{1}b = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix}$$
$$M_{2}M_{1}A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix}$$
$$M_{2}M_{1}b = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

Finally, solve the following system via back substitution.

$$\begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

Note that using the fact that the L matrices are inverses of the M matrices allows us to write $LU = (L_1 \dots L_{n-1})(M_{n-1} \dots M_1 A) = A$ where $L = L_1 \dots L_{n-1}$ can be formed trivially from the M_k to obtain:

$$L = L_1 L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix}$$

And thus, although we never needed it to solve the equations, the LU factorization of ${\cal A}$ is

$$A = \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} = LU$$

Existence/Uniqueness and pivoting

When computing the LU factorization, the algorithm will halt if the diagonal element $a_{kk} = 0$. This can be avoided by swapping rows of A prior to computing the LU factorization. This is done to always select the largest a_{kk} from the equations that follow. As an example, consider the matrix A and the action of the permutation matrix P on it.

$$A = \begin{bmatrix} 1 & 2 & 5 & -1 \\ 0 & 0 & 3 & 1 \\ 0 & 4 & 1 & -2 \\ 0 & -6 & 0 & 3 \end{bmatrix}, P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, PA = \begin{bmatrix} 1 & 2 & 5 & -1 \\ 0 & -6 & 0 & 3 \\ 0 & 4 & 1 & -2 \\ 0 & 0 & 3 & 1 \end{bmatrix}$$

This is pivoting: the pivot a_{kk} is selected to be non-zero. In this process, we can guarantee uniqueness and existence of LU:

Theorem 2. If P is a permutation matrix such that all pivots in the Gaussian Elimination of PA are non-zero, and $l_{ii} = 1$, then the LU factorization exists and is unique!

$$PA = LU$$