Linear system.

CS450: Numerical Analysis

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Solving Linear Systems

- For a square matrix $\boldsymbol{A}$, how to (systematically) solve for $\boldsymbol{Ax} = \boldsymbol{b}$?
  - Transform it into one whose solution is the same but easier to compute
  - Specifically, eliminate x_1 from $n-1$ equations to get a smaller system $\boldsymbol{A_2 x} = \boldsymbol{b_2}$ of size $n-1$
  - Eventually, reaching the 1 by 1 system $A_n x_n = b_n$ which we know $x_n = b_n / A_n$
  - Working backwards produces $x_{n-1}, x_{n-2}, \ldots,$ and eventually x_2 and x_1

$$
\begin{matrix}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\
a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\
\vdots \\
a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n
\end{matrix}
\Rightarrow
\begin{matrix}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\
\begin{matrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{matrix} \quad \boxed{\quad A_2 \quad} \; x = b_2
\end{matrix}
\Rightarrow \cdots \Rightarrow \boxed{A_n x_n = b_n}
$$

$$x_n = b_n / A$$

Triangular Linear Systems

- What type of linear system is easy to solve?
  - Systems that form triangular matrices

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= a_{1,n+1} \\
a_{22}x_2 + \cdots + a_{2n}x_n &= a_{2,n+1} \\
&\vdots \\
a_{nn}x_n &= a_{n,n+1}
\end{aligned}
$$

$A x = b$

$x = b$

$a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = a_{n-1,n+1}$

  - Back-substitution

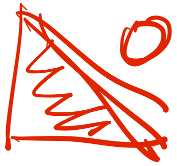
$$x_n = \frac{a_{n,n+1}}{a_{nn}},$$

$$x_i = \frac{a_{i,n+1} - \sum_{j=i+1}^{n} a_{ij}x_j}{a_{ii}}, \; i = n-1, \ldots, 1$$

Triangular Matrices

- Two specific triangular forms are of particular interest
  - Lower triangular: all entries above main diagonal are zero, $a_{ij} = 0$ for $i < j$
  - Upper triangular: all entries below main diagonal are zero, $a_{ij} = 0$ for $i > j$

$$
\begin{aligned}
a_{11}x_1 &= b_1 \\
a_{21}x_1 + a_{22}x_2 &= b_2 \\
\vdots \quad \ddots \quad & \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn} &= b_n
\end{aligned}
$$



$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{2n}x_n &= b_2
\end{aligned}
$$

Triangular Matrices (cont'd)

- Two specific triangular forms are of particular interest
  - Lower triangular: all entries above main diagonal are zero, $a_{ij} = 0$ for $i < j$
  - Upper triangular: all entries below main diagonal are zero, $a_{ij} = 0$ for $i > j$
- Successive substitution process described earlier is especially easy to formulate for lower or upper triangular systems
- Any triangular matrix can be permuted into upper or lower triangular form by suitable row permutation

Elimination

- To transform general linear system into triangular form, we need to replace selected nonzero entries of matrix by zeros
- This can be accomplished by taking linear combinations of rows
- Consider a two-dimensional vector $\boldsymbol{a} = [a_1\ a_2]$
- If $a_1 \neq 0$, then

$$\begin{bmatrix} 1 & 0 \\ -a_2/a_1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}$$

$\leftarrow 1 \times a_1 + 0 \times a_2 = a_1$

$\leftarrow \left(-\frac{a_2}{a_1}\right) \times a_1 + a_2 = -a_2 + a_2$

$= 0$

Elementary Elimination Matrices

$Ax=b \quad M_1Ax=M_1b \quad M_1 \rightarrow$

$A=[a_1\ a_2 \cdots a_n]$

$\det(A) \neq 0$

- More generally, we can annihilate all entries below k-th in a n-dimensional vector $\boldsymbol{a}$ by transformation

k-th column of I_n

$m_{k+1} = -\frac{a_{k+1}}{a_k}$

at the (k+1)-th column position

$m_{k+2} = -\frac{a_{k+2}}{a_k}$

$$\boldsymbol{M}_k\,\boldsymbol{a} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -m_n & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$(-m_{k+1}) \times a_k + 1 \times a_{k+1}$

$= -\frac{a_{k+1}}{a_k} \times a_k + a_{k+1} = 0$

where $m_i = \frac{a_i}{a_k}$, $i = k+1, \dots, n$

- Divisor a_k, called pivot, must be nonzero

Elementary Elimination Matrices (cont'd)

Example: For a vector $\boldsymbol{a} = [2, 4, -2]^T$, the elementary elimination matrices $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ are (recall: $m_i = \frac{a_i}{a_k}$, $i = k+1, \dots, n$)

$$-\frac{a_2}{a_1} = -\frac{4}{2} = -2$$

$$-\frac{a_3}{a_1} = -\frac{-2}{2} = 1$$

$$\boldsymbol{M}_1\boldsymbol{a} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

$$\boldsymbol{M}_2\boldsymbol{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$

Elementary Elimination Matrices (cont'd)

- Matrix $\boldsymbol{M}_k$, called elementary elimination matrix, adds multiple of row k to each subsequent row, with multipliers m_i chosen so that result is zero

- $\boldsymbol{M}_k$ is unit lower triangular and nonsingular

$[0\ 0 \dots 0\ 1\ 0 \dots 0]$ $\underbrace{\quad}_{(k-1)}$ k $(n-k+1)$

- $\boldsymbol{M}_k = \boldsymbol{I} - \boldsymbol{m}_k \boldsymbol{e}_k^T$, where $\boldsymbol{m}_k = [0, \dots, 0, m_{k+1}, \dots, m_n]^T$ and $\boldsymbol{e}_k$ is the k-th column of identity matrix

$\rightarrow$ outer product. rank-1

- $\boldsymbol{M}_k^{-1} = \boldsymbol{I} + \boldsymbol{m}_k \boldsymbol{e}_k^T$, which means $\boldsymbol{M}_k^{-1} = \boldsymbol{L}_k$ is the same as $\boldsymbol{M}_k$ except signs of multipliers are reversed

$$M_k M_k^{-1} = (I - m_k e_k^T)(I + m_k e_k^T)$$

$$= I + \cancel{m_k e_k^T} - \cancel{m_k e_k^T} - m_k e_k^T m_k e_k^T$$

$$e_k^T m_k = [\underbrace{0 \dots 0}_{(k-1)}\ \underset{k}{1}\ 0 \cdots 0] \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ m_{k+1} \\ \vdots \\ m_n \end{bmatrix} = 0$$

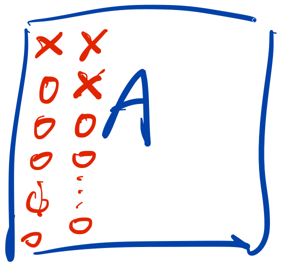
$$m_k \times 0 \times e_k^T = 0$$

$$M_k M_k^{-1} = I$$

Elementary Elimination Matrices (cont'd)

- If $\boldsymbol{M}_j$, $j > k$, is another elementary elimination matrix, with vectors of multipliers $\boldsymbol{m}_j$, then

$$\boldsymbol{M}_k\boldsymbol{M}_j = (\boldsymbol{I} - \boldsymbol{m}_k\boldsymbol{e}_k^T)(\boldsymbol{I} - \boldsymbol{m}_j\boldsymbol{e}_j^T)$$
$$= \boldsymbol{I} - \boldsymbol{m}_k\boldsymbol{e}_k^T - \boldsymbol{m}_j\boldsymbol{e}_j^T + \boldsymbol{m}_k\boldsymbol{e}_k^T\boldsymbol{m}_j\boldsymbol{e}_j^T$$
$$= \boldsymbol{I} - \boldsymbol{m}_k\boldsymbol{e}_k^T - \boldsymbol{m}_j\boldsymbol{e}_j^T$$



$M_1 M_2 \cdots$

where means product is essentially "union", and similarly for product of inverses, $\boldsymbol{L}_k\boldsymbol{L}_j$

Gaussian Elimination

$$\begin{bmatrix} 1 & & & \\ m_1 & 1 & & \\ m_2 & & \ddots & \\ \vdots & & & \\ m_n & & & 1 \end{bmatrix} = M_1$$

- To reduce a general linear system of equations $\boldsymbol{Ax} = \boldsymbol{b}$ into upper triangular form, do the following

$$M_2 M_1 A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & & \\ \vdots & 0 & & \\ 0 & 0 & \cdots & \end{bmatrix}$$

  - Choose $\boldsymbol{M}_1$ with a_{11} as pivot, annihilate first column of $\boldsymbol{A}$ below first row: the system becomes $\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_1\boldsymbol{b}$, but solution remains unchanged
  - Next choose $\boldsymbol{M}_2$ with a_{22} as pivot, annihilate second column of $\boldsymbol{M}_1\boldsymbol{A}$ below second row: the system becomes $\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{b}$, but the solution still unchanged
  - Process continues for each successive column until all subdiagonal entries have been zeroed, results in upper triangular linear system $\boldsymbol{M}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{b}$, which can be solved via back-substitution

- This process is called Gaussian elimination

LU Factorization

$M_{n-1}M_{n-2}\cdots M_2 M_1 A =$

$I + m_k e_k^T$

- Denote by $\boldsymbol{M}_k^{-1} = \boldsymbol{L}_k$, then $\boldsymbol{L} = \boldsymbol{M}^{-1} = \boldsymbol{M}_1^{-1}\cdots\boldsymbol{M}_{n-1}^{-1} = \boldsymbol{L}_1\cdots\boldsymbol{L}_{n-1}$ is lower triangular $(M_{n-1}\cdots M_1)^{-1}U = A$

$M_{n-2}^{-1}M_{n-1}^{-1}U = M_{n-3}\cdots M_1 A$

- By design, $\boldsymbol{U} = \boldsymbol{M}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{A}$ is upper triangular
- Therefore, we can factorize matrix $\boldsymbol{A}$ into the product of a lower triangular matrix and an upper triangular matrix

$A = M_1^{-1}M_2^{-1}\cdots M_{n-1}^{-1}U$

$= LU$

$Ax = b_1 \qquad Ax = b_2$

$LUx = b_1 \to Ux = L^{-1}b_1$

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$$

- Thus, Gaussian elimination produces LU factorization of matrix into triangular factors

$Ax = \boxed{b} \Rightarrow MAx = Mb \Rightarrow A = LU$

Fourier Transform

LU Factorization (cont'd)

- The LU factorization can be viewed as a sum of rank-1 matrices

$$A = \begin{bmatrix} 1 \times \bar{r}_1 \\ -m_{21} \times \bar{r}_1 \\ -m_{31} \times \bar{r}_1 \\ \vdots \\ -m_{n1} \times \bar{r}_1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & & & & \\ 0 & & \boxed{A_2} & & \\ \vdots & & & & \\ 0 & & & & \end{bmatrix} = \bar{m}_1 \times \bar{r}_1 + \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \boxed{A_2} & \\ 0 & & & \end{bmatrix}$$

$$+ \bar{m}_i \times \bar{r}_i + \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & 0 & & \\ \vdots & \vdots & \boxed{A_3} & \end{bmatrix}$$

LU Factorization (cont'd)

$Ax=b \rightarrow A=LU$

- With LU factorization, the linear system becomes $\boldsymbol{LUx} = \boldsymbol{b}$

$Ux=y$

$\rightarrow Ly=b$

- Can be solved by forward-substitution in lower triangular system $\boldsymbol{Ly} = \boldsymbol{b}$
- Followed by back-substitution $\boldsymbol{Ux} = \boldsymbol{y}$ in upper triangular system
- Gaussian elimination and LU factorization are two ways of expressing same solution process
- What's the advantage of LU factorization?

$$
\begin{aligned}
a_{11}y_1 &= b_1\\
a_{12}y_1 + a_{12}y_2 &= b_2\\
&\vdots\\
a_{n1}y_1 + a_{n2}y_2 + \cdots + a_{nn}y_n &= b_n
\end{aligned}
$$

if $Ax=b$ is all I need.

if $Ax=b_1$

$Ax=b_2$

$\vdots$

$Ax=b_k$ ...

$$
\begin{aligned}
u_{11}x_1 + u_{12}x_2 + \cdots + u_{1n}x_n &= y_1\\
u_{22}x_2 + \cdots + u_{2n}x_n &= y_2\\
&\vdots\\
u_{nn}x_n &= y_n
\end{aligned}
$$

Working Example

- Apply Gaussian elimination to the following system using four-digit arithmetic with rounding, and compare the result to the exact solution $x_1 = 10.00$ and $x_2 = 1.000$

$$M_1 = \begin{bmatrix} 1 & 0 \\ -m_1 & 1 \end{bmatrix} \qquad -m_1 = -\frac{a_{21}}{a_{11}}$$

$$= -\frac{5.291}{0.003000}$$

$$= -1763.6\overline{6}$$

$$\approx -1764$$

$$E_1: \quad 0.003000x_1 + 59.14x_2 = 59.17$$
$$E_2: \quad 5.291x_1 - 6.130x_2 = 46.78.$$

$$\begin{bmatrix} 1 & 0 \\ -1764 & 1 \end{bmatrix} \times A x = \begin{bmatrix} 1 & 0 \\ -1764 & 1 \end{bmatrix} b$$

Working Example

$$A = \begin{bmatrix} 0.003 & 59.14 \\ 5.291 & -6130 \end{bmatrix}$$

$$K(A) \simeq 11.2982$$

- Gaussian elimination using four-digit arithmetic with rounding

$$\begin{aligned} E_1 : \quad & 0.003000x_1 + 59.14x_2 = 59.17 \\ E_2 : \quad & 5.291x_1 - 6.130x_2 = 46.78 \end{aligned}$$

$$5.291x_1 - 6.130x_2 = 46.78$$

$$0.003x_1 + 59.14x_2 = 59.17$$

$$0.00300x_1 + 59.14x_2 = 59.17$$

$$-104300x_2 = -104400$$

$$x_2 \approx \frac{-104400}{-104300} \approx 1.001$$

$$x_1 = \frac{59.17 - 59.14 \times 1.001}{0.00300} = -10.00$$

Partial Pivoting

- In principle, any nonzero value can serve as the pivot
- In practice, chose the one that minimizes error propagation
- Approach: select an element in the same column that is below the diagonal and has the largest absolute value

$$a_{11}x_1 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + \cdots$$
$$\vdots$$
$$a_{n1}x_1 + \cdots$$

Working Example (cont'd)

- Apply Gaussian elimination to the following system using partial pivoting and four-digit arithmetic with rounding, and compare the result to the exact solution $x_1 = 10.00$ and $x_2 = 1.000$

$$
\begin{aligned}
E_1: &\quad 0.003000x_1 + 59.14x_2 = 59.17 \\
E_2: &\quad 5.291x_1 - 6.130x_2 = 46.78.
\end{aligned}
$$