# Numerical linear algebra (20)

## 20.1 Gauss elimination

The goal is to solve a linear system of $n$ equations:

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

$$\vdots$$

$$a_{n1}x_1 + \cdots + a_{nn}x_n = b_n$$

$$Ax = b$$

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

$\tilde{A}$ augmented matrix

$= [A \quad b]$

Example:

$$0.0004x_1 + 1.402x_2 = 1.406$$
$$0.4003x_1 - 1.502x_2 = 2.501$$

We want to see the bad behavior of roundoff error when $|a_{11}| \ll |a_{21}|$.

Solution $x_1 = 10$, $x_2 = 1$.

Gauss elimination

$$\left(\begin{array}{cc|c} 0.0004 & 1.402 & 1.406 \\ 0.4003 & -1.502 & 2.501 \end{array}\right)$$

$0.4003 \leftarrow 0$

$$L_2 \longrightarrow L_2 - \frac{0.4003}{0.0004} L_1$$

$$= L_2 - 1001\, L_1$$

$$\left(\begin{array}{cc|c} 0.0004 & 1.402 & 1.406 \\ 0 & -1405 & -1404 \end{array}\right)$$

$$\Rightarrow x_2 = -1404 / -1405$$

$X_2 = 0.9993$

$0.0004 x_1 + 1.402 \cdot 0.9993 = 1.406$

$\Rightarrow x_1 = \frac{1}{0.0004}(1.406 - 1.402 \cdot 0.9993)$

$= 12.5$. BAD

This occurs because $|a_{11}| << |a_{12}|$.

<u>Strategy</u>: Swap the two rows (Want the pivot to be the biggest)

If we had exchanged the row, then

$$L_2 \longrightarrow L_2 - 0.0009993 L_1$$

$$1.404 x_2 = 1.404 \Rightarrow x_2 = 1$$

& $x_1 = 10$.

## Gauss elimination algorithm

Input: augmented matrix

$$\tilde{A} = [\underset{n\times n}{A} \quad \underset{n+1 \text{ column}}{b}]$$

1) Swap the rows so that the pivot is the biggest.

For $k = 1, \ldots, n-1$ do:

$m = k$

For $j = k+1 \dots n$

If $(|a_{mk}| < |a_{jk}|)$

then $m = j$.

End If $a_{mk} = 0 \Rightarrow$ Stop

Exchange row $k$ and row $m$

2) Gauss elimination

For $j = k+1, \dots, n$ do

$m_{jk} := \frac{a_{jk}}{a_{kk}}$ (multiplier)

$\hookrightarrow$ pivot

For $p = k+1 \dots n+1$

$$a_{jp} := \underbrace{a_{jp} - m_{jk} a_{kp}}_{\text{Subtracting two rows}}$$

End

End

End

3) Back substitution

If $a_{nn} = 0$ STOP

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

For $i = n-1, \dots, 1$ do

$$x_i = \frac{1}{a_{ii}}\left(a_{i,n+1} - \sum_{j=i+1}^{n} a_{ij} x_j\right)$$

End

Example:

$$\begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \left(\begin{array}{ccc|c} -3 & 6 & -9 & -46.725 \\ 1 & -4 & 3 & 19.571 \\ 2 & 5 & -7 & -20.073 \end{array}\right) \end{array}$$

1) Swap rows

$k=1, \quad m=1$

$|a_{11}| \not< |a_{21}|, \quad |a_{11}| \not< |a_{31}|$

No swap. $\Rightarrow m=1$

$a_{11} \neq 0$ ✓

2) Gauss elimination

$$m_{21} = \frac{a_{21}}{a_{11}} = \frac{1}{-3} = -0.33333$$

$$m_{31} = \frac{a_{31}}{a_{11}} = \frac{2}{-3} = -0.66667$$

For $p = 2 \ldots 4$

$L_2 \rightarrow L_2 - m_{21} L_1$ (term by term)

$L_3 \rightarrow L_3 - m_{31} L_1$

End

$$\left(\begin{array}{ccc|c} -3 & 6 & -9 & -46.725 \\ 0 & -2.1000 & 0.00003 & 3.9962 \\ 0 & 9.0000 & -13.000 & -51.223 \end{array}\right)$$

↳ $k=2$ $m=2$

1) Swap $L_3$ & $L_2$

because $|a_{22}| < |a_{32}|$.

$$\left(\begin{array}{ccc|c} -3 & 6 & -9 & -46.725 \\ 0 & 9. & -13. & -51.223 \\ 0 & -2. & 0.00003 & 3.9962 \end{array}\right)$$

0

2) Gauss elimination

$$m_{23} = \frac{a_{32}}{a_{22}} = -0.22222$$

$$L_3 \longrightarrow L_3 - m_{23} L_2$$ (term by term)

$$\left(\begin{array}{ccc|c} -3 & 6 & -9 & -46.725 \\ 0 & 9 & -13 & -51.223 \\ 0 & 0 & -2.88883 & -7.3866 \end{array}\right)$$

End

3) Back substitution

$$-3x_1 + 6x_2 - 9x_3 = -46.725$$

$$9x_2 - 13x_3 = -51.223$$

$$-2.88883x_3 = -7.3866$$

$$x_3 = \frac{a_{34} \leftarrow b_3}{a_{33}} = \frac{-7.3866}{-2.88883} = \boxed{2.557}$$

$$x_2 = \frac{1}{9}\left(-51.223 + 13 \cdot x_3\right)$$

$$= \boxed{-1.998}$$

$$x_1 = -\frac{1}{3}\left(-46.725 - 6 \cdot x_2 + 9x_3\right)$$

$$\boxed{= 3.908}$$

End.

## Operation count

~ how much times the algorithm takes

$(+, -, \times, \div)$

**Gauss elimination**: step $k$

multipliers $(n-k)$ division:

$L_j \to L_j - m_{kj} L_k$

sub. multi

$\underbrace{(n-k)}_{\text{rows}} \underbrace{(n-k+1)}_{\text{columns}}$ multiplications & substractions

In total:

$$f(n) = \sum_{k=1}^{n-1}(n-k) + 2\sum_{k=1}^{n-1}(n-k)(n-k+1)$$

$\parallel$

# operations

$$= \frac{1}{2}(n-1)n + \frac{2}{3}(n^2-1)n$$

$$\approx \frac{2}{3}n^3$$

$$= O(n^3), \text{ which}$$

means

$$0 < \lim_{n\to\infty} \frac{|f(n)|}{|n^3|} < \infty$$

Back substitution: step $i$

$$x_i = \frac{1}{a_{ii}}\left(a_{i,n+1} - \sum_{j=i+1}^{n} a_{ij}x_j\right)$$

1 division

$n-i$ substractions

$n-i$ mult.

$\Rightarrow 2(n-i)+1$ operations

In total,

$$b(n) = 2\sum_{i=1}^{n}(n-i) + \sum_{i=1}^{n} 1$$

$$= n^2 + 2n = O(n^2)$$

If an operation takes $10^{-9}$ sec

$n = 10\,000$

$\Rightarrow$ 11 min Gauss elim.

0.1 sec Back subst.

<u>LU-factorization</u> (20.2)

Advantage: no Gauss elimin.

faster $\sim \frac{1}{3} n^3$ operations

An LU-factorization of a given square matrix A

$$A = L\,U$$

lower triang. | upper triangular

If A is invertible, then can always reorder the rows so that LU-factoriz. exists.

Can also ask for the diagonal elements in L or U to be 1's.

Want to solve

$$Ax = b$$

$$\Rightarrow \underbrace{LUx}_{y} = b$$

1. $Ly = b$
2. $Ux = y$

$L, U$ are triangular $\Rightarrow$ very fast (back substitution)

$x$ ← Solution.

Doolittle's method

$L$ has 1's in the diagonal.

Example:

$$\left(\underbrace{\begin{matrix} 5 & 4 & 1 \\ 10 & 9 & 4 \\ 10 & 13 & 15 \end{matrix}}_{A} \;\middle|\; \underbrace{\begin{matrix} 6.8 \\ 17.6 \\ 38.4 \end{matrix}}_{B}\right)$$

1) $A = LU$

$$\begin{pmatrix} 5 & 4 & 1 \\ 10 & 9 & 4 \\ 10 & 13 & 15 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ m_{21} & 1 & 0 \\ m_{31} & m_{32} & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

$u_{11} = 5 \qquad u_{12} = 4 \qquad u_{13} = 1$

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$m_{21} \cdot u_{11} = 10 \Rightarrow m_{21} = 2$

$m_{21} u_{12} + 1 \cdot u_{22} = 9 \Rightarrow u_{22} = 1$

$m_{21} \cdot u_{13} + 1 \cdot u_{23} = 4 \Rightarrow u_{23} = 2$

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$m_{31} \cdot u_{11} = 10 \Rightarrow m_{31} = 2$

$m_{31} \cdot u_{12} + m_{32} \cdot u_{22} = 13 \Rightarrow m_{32} = 5$

$m_{31} u_{13} + m_{32} \cdot u_{23} + 1 \cdot u_{33} = 15$

$\Rightarrow u_{33} = 3$

$$\begin{pmatrix} 5 & 4 & 1 \\ 10 & 9 & 4 \\ 10 & 13 & 15 \end{pmatrix} = \underset{L}{\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 5 & 1 \end{pmatrix}} \underset{U}{\begin{pmatrix} 5 & 4 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & 3 \end{pmatrix}}$$

1) Solve $Ly = b$ by "back" substitution

$$y_1 = b_1 \Rightarrow y_1 = 6.8$$

$$2y_1 + y_2 = b_2 \Rightarrow y_2 = 4$$

$$2y_1 + 5y_2 + y_3 = b_3 \Rightarrow y_3 = 4.8$$

2) $Ux = y$ by back substitution

$$5x_1 + 4x_2 + x_3 = 6.8$$
$$x_2 + 2x_3 = 4$$
$$3x_3 = 4.8$$

$$\Rightarrow \boxed{x = \begin{pmatrix} 0.4 \\ 0.8 \\ 1.6 \end{pmatrix}}$$

Formulas for the entries of $L = [m_{jk}]$ (diagonal $= 1, \dots 1$)

$U = [u_{jk}]$

1) $u_{1k} = a_{1k} \quad k = 1, \dots, n$

2) $m_{j1} = \dfrac{a_{j1}}{u_{11}} \quad j = 2, \dots, n$

3) $u_{jk} = a_{jk} - \sum_{s=1}^{j-1} m_{js} u_{sk} \quad k = j \dots n$
$j \geq 2$

4) $m_{jk} = \dfrac{1}{u_{kk}} \left( a_{jk} - \sum_{s=1}^{k-1} m_{js} u_{sk} \right)$

$j = k+1, \ldots, n$ ; $k \geq 2$

Be careful!

$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$ does not have LU factorization

Need to swap rows.