Workshop 4
Linear Systems

FIT 3139

Computational Modelling and Simulation

MONASH University
Information Technology

Linear system

$$A\vec{x} = \vec{b} \quad ?$$

General elimination matrix

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

$$a_k \neq 0 \qquad\qquad m_i = \frac{a_i}{a_k} \forall k < i \leq n$$

a_k is know as the common **pivot**

Elementary Elimination Matrix

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ -\frac{a_2}{a_1} & 1 & 0 \\ -\frac{a_3}{a_1} & 0 & 1 \end{pmatrix}}_{\text{Elimination matrix}} \underbrace{\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}}_{\text{Column vector}} = \underbrace{\begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix}}_{\text{column vector with eliminated terms}}$$

$$A\vec{x} = \vec{b} \quad \xrightarrow{\text{GOAL}} \quad U\vec{x} = \vec{z}$$

$$M_1 A\vec{x} = M_1\vec{b}$$

Build M_1 using elements in first column of A

Eliminate terms below first diagonal element

$$M_2 M_1 A\vec{x} = M_2 M_1\vec{b}$$

Eliminate terms below second diagonal element

$$\vdots$$

$$M_{n-1} \ldots M_2 M_1 A\vec{x} = M_{n-1} \ldots M_2 M_1\vec{b}$$

$$U\,\vec{x} = \vec{z}$$

backward substitution

Properties of Elementary Elimination Matrices

M_k is **non-singular** (the diagonal is made of 1 and it is lower triangular).

M_k^{-1} is the same as M_k except the s**igns of the multipliers are reversed**.

$M_k M_j$ is “the union” of M_k and M_j , provided $j > k$.

This is amazing!

$$\overbrace{\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}}^{A} \overbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}}^{x} = \overbrace{\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}}^{b}$$

$$\overbrace{\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix}}^{U} \overbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}}^{x} = \overbrace{\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}}^{z}$$

$$\begin{aligned}
u_{44}x_4 = z_4 &\implies & x_4 &= \frac{z_4}{u_{44}} \\
u_{33}x_3 + u_{34}x_4 = z_3 &\implies & x_3 &= \frac{z_3 - u_{34}x_4}{u_{33}} \\
u_{22}x_2 + u_{23}x_3 + u_{24}x_4 = z_1 &\implies & x_2 &= \frac{z_2 - u_{23}x_3 - u_{24}x_4}{u_{22}} \\
u_{11}x_1 + u_{12}x_2 + u_{13}x_3 + u_{14}x_4 = z_1 &\implies & x_1 &= \frac{z_1 - u_{12}x_2 - u_{13}x_3 - u_{14}x_4}{u_{11}}
\end{aligned}$$

For a **lower triangular** matrix we have a similar **forward substitution** procedure.

Algorithm 1 Back substitution for upper triangular system

BACK-SUBSTITUTION(U, z)

for j in $\{n, \cdots, 1\}$: ▷ Loop backwards over columns
  do
    if $u_{jj} = 0$
      then Stop ▷ Stop if matrix is singular
    $x_j = \frac{z_j}{u_{jj}}$ ▷ Compute solution component
    for i in $\{1, \cdots, j-1\}$:
      do
        $z_i = z_i - u_{ij}x_j$ ▷ Update rigth-hand side

Let's go **back to the task**

(transforming the problem into an easy one)

Example

$$x_1 + 2x_2 + 2x_3 = 3$$
$$4x_1 + 4x_2 + 2x_3 = 6$$
$$4x_1 + 6x_2 + 4x_3 = 10$$

$$Ax = b$$

$$\boxed{\begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \\ 10 \end{pmatrix}}$$

$$M_1 A = \begin{pmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{pmatrix}$$

$$M_1 b = \begin{pmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 6 \\ 10 \end{pmatrix} = \begin{pmatrix} 3 \\ -6 \\ -2 \end{pmatrix}$$

$$\boxed{\begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -6 \\ -2 \end{pmatrix}}$$

$$\begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -6 \\ -2 \end{pmatrix}$$

Gaussian elimination
= Forward elimination + Back substitution

$$M_2 M_1 A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.5 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{pmatrix}$$

$$M_2 M_1 b = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -0.5 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ -6 \\ -2 \end{pmatrix} = \begin{pmatrix} 3 \\ -6 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ -6 \\ 1 \end{pmatrix}$$

backward substitution

$$U \vec{x} = \vec{z}$$

LU factorisation

$$Ax = b$$

$$\underbrace{M_{n-1}\ldots M_1 A}_{\text{Upper triangular}}x = \underbrace{M_{n-1}\ldots M_1}_{\text{Lower triangular}}b$$

$$(M_{n-1}\ldots M_1)^{-1}(M_{n-1}\ldots M_1)Ax = b$$

$$(M_1^{-1}M_2^{-1}\ldots M_{n-1}^{-1})(M_{n-1}\ldots M_1)Ax = b$$

$$\underbrace{(L_1L_2\ldots L_{n-1})}_{\text{Lower triangular}}\underbrace{(M_{n-1}\ldots M_1)A}_{\text{Upper triangular}}x = b$$

$$L\ U\ x = b$$

A turns into **L** and **U**

$$Ax = b$$

$$L\ U\ x = b$$

$$L\ y = b$$

known

known

~~unknown~~

known!

$$Ux = y$$

n x 1 unknown

forward substitution

backward substitution

DONE!

Summary…

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Forward elimination

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = M_3 M_2 M_1 \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

$$M_1^{-1} M_2^{-1} M_3^{-1} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Summary…

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Forward elimination

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = M_3 M_2 M_1 \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

$$\begin{pmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{23} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Summary…

$$\begin{pmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{23} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

$$\begin{pmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{23} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Forward substitution to find **y**

$$\begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}$$

Backward substitution to find **x**

Which is better?

HOMEWORK

Potential issues

- Division by zero
- Round-off error

$$\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 3.901 \\ 6 \end{pmatrix}$$

6 significant digits

with chopping

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15005 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 6.001 \\ 15005 \end{pmatrix}$$

$$x_3 = 1$$

$$x_2 = -1$$

$$x_1 = 0$$

5 significant digits

with chopping

$$\begin{pmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15004 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 6.001 \\ 15005 \end{pmatrix}$$

$$x_3 = 0.99993$$

$$x_2 = -1.5$$

$$x_1 = -0.35$$

Smaller pivots $\longrightarrow$ Larger multiplier $\longrightarrow$ Large error

Larger pivots $\longrightarrow$ Smaller multiplier $\longrightarrow$ Smaller error

In a column, if you **use the largest entry on or below the diagonal as the pivot**… then multipliers are bounded by 1

Use a permutation matrix to swap rows… $\longrightarrow$ **Partial pivoting**

$$Ax = \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \\ 10 \end{pmatrix} = b$$

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

$$P_1 Ax = \begin{pmatrix} 4 & 4 & 2 \\ 1 & 2 & 2 \\ 4 & 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 3 \\ 10 \end{pmatrix} = P_1 b$$

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

$$M_1 P_1 Ax = \begin{pmatrix} 4 & 4 & 2 \\ 0 & 1 & 1.5 \\ 0 & 2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 1.5 \\ 4 \end{pmatrix} = M_1 P_1 b$$

$$M_1P_1Ax = \begin{pmatrix} 4 & 4 & 2 \\ 0 & 1 & 1.5 \\ 0 & 2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 1.5 \\ 4 \end{pmatrix} = M_1P_1b$$

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

$$P_2M_1P_1Ax = \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 1 & 1.5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \\ 1.5 \end{pmatrix} = P_2M_1P_1b$$

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

$$M_2P_2M_1P_1Ax = \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \\ -0.5 \end{pmatrix} = M_2P_2M_1P_1b$$

$$M_2P_2M_1P_1Ax = \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \\ -0.5 \end{pmatrix} = M_2P_2M_1P_1b$$

For explicit **LU** decomposition

$$L = M^{-1} = (M_2P_2M_1P_1)^{-1} = \quad P_1^TL_1P_2^TL_2 = \begin{pmatrix} 0.25 & 0.5 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} = \begin{pmatrix} 0.25 & 0.5 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{pmatrix} = LU$$

But L is not lower triangular! 😱

$$P = P_2P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

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

$$PA = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0.25 & 0.5 & 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & 0.5 \end{pmatrix} = LU$$

$$PA = LU$$

Partial pivoting… extra (thin) layer of complexity, with permutations….

scipy.linalg.lu

scipy.linalg.lu(*a*, *permute_l=False*, *overwrite_a=False*, *check_finite=True*) [source]

Compute pivoted LU decompostion of a matrix.

The decomposition is:

```
A = P L U
```

where P is a permutation matrix, L lower triangular with unit diagonal elements, and U upper triangular.

Parameters:

a : *(M, N) array_like*
Array to decompose

permute_l : *bool*
Perform the multiplication P*L (Default: do not permute)

overwrite_a : *bool*
Whether to overwrite data in a (may improve performance)

check_finite : *boolean, optional*
Whether to check that the input matrix contains only finite numbers. Disabling may give a performance gain, but may result in problems (crashes, non-termination) if the inputs do contain infinities or NaNs.

Returns:

(If permute_l == False)

p : *(M, M) ndarray*
Permutation matrix

l : *(M, K) ndarray*
Lower triangular or trapezoidal matrix with unit diagonal. K = min(M, N)

u : *(K, N) ndarray*
Upper triangular or trapezoidal matrix

(If permute_l == True)

pl : *(M, K) ndarray*
Permuted L matrix. K = min(M, N)

u : *(K, N) ndarray*
Upper triangular or trapezoidal matrix

Previous topic

scipy.linalg.eigvals_banded

Next topic

scipy.linalg.lu_factor

https://docs.scipy.org/doc/scipy-0.14.0/reference/generated/scipy.linalg.lu.html