Boundary value problem

- Our case in Pr. 1 : $- \frac{d^2u}{dx^2} = f(x)$ $x \in [0,1]$

  - $u(x)$ unknown
  - $f(x)$ known
  - $x \in [0,1]$
  - Boundary values : $u(0) = 0$, $u(1) = 0$ (Dirichlet)

- Special case of :

$$\alpha \frac{d^2u}{dx^2} + \beta \frac{du}{dx} + \gamma u(x) = f(x)$$

  - Ordinary diff. eq. (only one indep. variable x)
  - Linear diff. eq. (each term has max. one power of $u, u', u'', \ldots$)
  - Second order (highest-order derivative is u'')
  - Inhomogenous ($f(x) \neq 0$)

- Most diff. eqs. in physics are linear. $\Rightarrow$ sum of two solutions is a new valid solution!

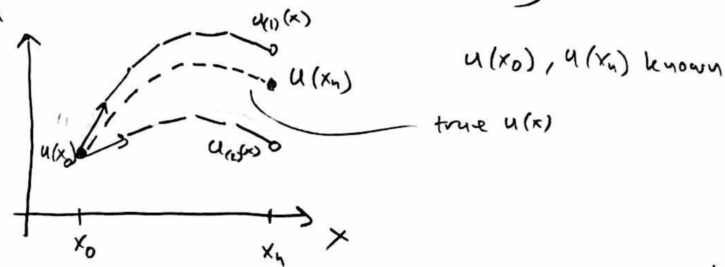
  Most famous example

  Schr. eq. in QM is linear

  ↳ Superposition of quantum states!

- Many approaches :
  - Shooting methods (quickly disc.)
  - Finite diff. methods (Pr. 1)
  - Finite elem. methods (not covered)

- Shooting method intuition
  - Turn B.V.P. into initial value problem (know $u(x_0)$ and $u'(x_0)$)
  - Know $u(x_0)$
  - Guess $u'(x_0)$ and solve forward ("shoot")
    $\rightarrow$ one attempt $u_{(1)}(x)$
  - Guess another $u'(x_0)$ and solve forward
    $\rightarrow$ second attempt $u_{(2)}(x)$
  - Sum of solutions is a new solution (linearity)
    $u_c(x) = c\, u_{(1)}(x) + (1-c)\, u_{(2)}(x)$
  - Require that $u_c(x_n) = u(x_n)$ (second bound. cond.) $\Rightarrow$ Determines c $\Rightarrow$ Solution $u(x) = u_c(x)$!



Finite diff. method

- We have: $-\frac{d^2u}{dx^2} = f(x)$
- Goal: Find $u(x)$
- Know: $x \in [0,1]$, $u(0)$, $u(1)$, $f(x)$
- Strategy: (1) Express as matrix eq.
  (2) Solve matrix eq.

(1) Express as matrix eq.

- Discretize

$$-\left[\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^2)\right] = f_i \qquad f_i \equiv f(x_i)$$

- Approximate
- Change notation: $v_i \approx u_i$

$$-\left(\frac{v_{i+1} - 2v_i + v_{i-1}}{h^2}\right) = f_i$$

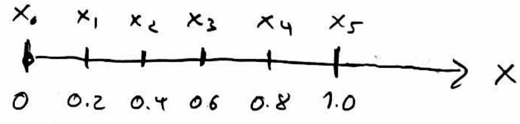
- Arrange terms

$$(*) \quad \boxed{-v_{i-1} + 2v_i - v_{i+1} = h^2 f_i}$$

Goal: Determine $v_1, v_2, .., v_{n-1}$
Know: v_0, v_n, all f_i

- Here: $n_{steps} = 5$
  $v_0, v_1, v_2, v_3, v_4, v_5$: 6 pts
  v_0, v_5 are boundary pts.
  4 unknown: $v_1, .., v_4$

Pr 1: You will generalize this!



$h = 0.2$ (very large...)

- (*) represents a set of eqs. Let's write them out in a suggestive way!

$$
\begin{array}{llllll}
(i=1) & -v_0 + 2v_1 - v_2 & & & & = h^2 f_1 \\
(i=2) & & -v_1 + 2v_2 - v_3 & & & = h^2 f_2 \\
(i=3) & & & -v_2 + 2v_3 - v_4 & & = h^2 f_3 \\
(i=4) & & & & -v_3 + 2v_4 - v_5 & = h^2 f_4
\end{array}
$$

- v_0, v_5 are known

define notation ↓

$$
\begin{array}{lllll}
2v_1 - v_2 & & & = h^2 f_1 + v_0 & \equiv g_1 \\
-v_1 + 2v_2 - v_3 & & & = h^2 f_2 & \equiv g_2 \\
& -v_2 + 2v_3 - v_4 & & = h^2 f_3 & \equiv g_3 \\
& & -v_3 + 2v_4 & = h^2 f_4 + v_5 & \equiv g_4
\end{array}
$$

- Can be written as

$$
\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}
\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}
=
\begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix}
$$

$$\boxed{A\bar{v} = \bar{g}}$$

- A, $\bar{g}$ known
- Want to solve for $\bar{v}$

(2) Solve matrix eq.

- Overview of things we'll discuss

1) Solving a <u>general</u> matrix eq. $A\bar{v} = \bar{g}$

(Gauss elim., LU decomp., iterative methods, ...)

Now $\rightarrow$ 2) Solving $A\bar{v} = \bar{g}$ when A is a <u>general tridiagonal</u> matrix

<u>Gauss elim.</u> $\Rightarrow$ Thomas algorithm

3) Solving $A\bar{v} = \bar{g}$ when A is the special tridiag. matrix

$$A = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & 0 \\ & -1 & 2 & -1 \\ 0 & & \ddots & \ddots \end{bmatrix}$$

superdiag.

subdiag. main diag

(You'll think about this in Pr. 1)

- First some words about matrix eq. ...

About solving matrix eqs.

$$\boxed{A\bar{x}=\bar{b}}$$

$A, \bar{b}$ known
$\bar{x}$ unknown

- Comes from set of linear equations

$$\text{m eqs.}\left\{\begin{array}{l} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2 \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n = b_m \end{array}\right.$$

n terms, one per unknown variable $(x_1, x_2, \ldots, x_n)$

- In general:

$$\underset{(m\times n)}{A}\ \underset{(n\times 1)}{\bar{x}} = \underset{(m\times 1)}{\bar{b}}$$

e.g.

$$\underset{(4\times 3)}{\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{bmatrix}} \underset{(3\times 1)}{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}} = \underset{(4\times 1)}{\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}}$$

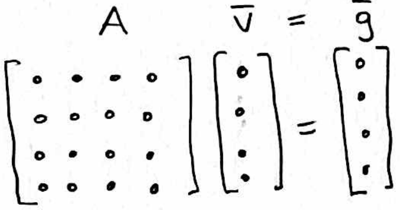
- We'll focus on the case $m=n \iff A$ is square
$\iff n$ eqs. and n unknowns

- If all eqs. are lin. indep. (each eq. represent info not contained in the other eqs.) we should be able to solve for all unknowns $(x_1, \ldots, x_n)$, i.e. for $\bar{x}$.

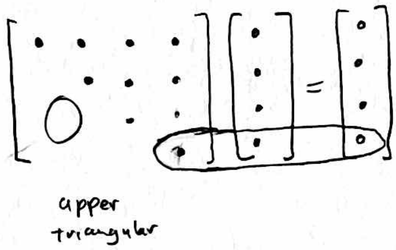
[If you have more eqs. than unknowns
$\rightarrow$ no exact solution, but can fit unknowns. Typical case in science!]

- All eqs. are lin. indep. $\iff$ A is not singular $\iff$ $\det(A) \neq 0$
(all eigenvalues of A are $\neq 0$)

- Gaussian elimination

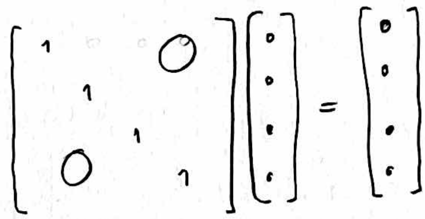


- step 1 : Forward subst. / elimin.
  [Turn into upper triang. form] $\Rightarrow$



trivial to solve for last v_i

- step 2 : Back subst.
  [Use solution for v_i to find v_{i-1}] $\Rightarrow$



solved for all v_i

- Our case : General tridiagonal A (Gauss. elim. $\rightarrow$ Thomas algo.)

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 \\ 0 & a_3 & b_3 & c_3 \\ 0 & 0 & a_4 & b_4 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix}$$

subdiag: $\bar{a} = [a_2, a_3, a_4]$
main diag: $\bar{b} = [b_1, b_2, b_3, b_4]$
superdiag: $\bar{c} = [c_1, c_2, c_3]$

$$\begin{array}{lcccc|c} (R_1) & b_1 & c_1 & 0 & 0 & g_1 \\ (R_2) & a_2 & b_2 & c_2 & 0 & g_2 \\ (R_3) & 0 & a_3 & b_3 & c_3 & g_3 \\ (R_4) & 0 & 0 & a_4 & b_4 & g_4 \end{array}$$

$$\boxed{R_2 \rightarrow R_2 - \frac{a_2}{b_1} R_1}$$

$(a_2 - \frac{a_2}{b_1} b_1)$

$$\begin{array}{cccc|c} b_1 & c_1 & 0 & 0 & g_1 \\ 0 & (b_2 - \frac{a_2}{b_1} c_1) & c_2 & 0 & (g_2 - \frac{a_2}{b_1} g_1) \\ 0 & a_3 & b_3 & c_3 & g_3 \\ 0 & 0 & a_4 & b_4 & g_4 \end{array}$$

- New notation:
  - $\tilde{b}_2 = b_2 - \frac{a_2}{\tilde{b}_1} c_1$
  - $\tilde{g}_2 = g_2 - \frac{a_2}{\tilde{b}_1} \tilde{g}_1$

Also: $\tilde{b}_1 = b_1$

$\tilde{g}_1 = g_1$

$$
\left[\begin{array}{cccc|c}
\tilde{b}_1 & c_1 & 0 & 0 & \tilde{g}_1 \\
0 & \tilde{b}_2 & c_2 & 0 & \tilde{g}_2 \\
0 & a_3 & b_3 & c_3 & g_3 \\
0 & 0 & a_4 & b_4 & g_4
\end{array}\right]
$$

- Cont. like this:

Row op: $R_3 \rightarrow R_3 - \frac{a_3}{b_2} R_2$

Define:
- $\tilde{b}_3 = b_3 - \frac{a_3}{\tilde{b}_2} c_2$
- $\tilde{g}_3 = g_3 - \frac{a_3}{\tilde{b}_2} \tilde{g}_2$

$$
\left[\begin{array}{cccc|c}
\tilde{b}_1 & c_1 & 0 & 0 & \tilde{g}_1 \\
0 & \hat{b}_2 & c_2 & 0 & \hat{g}_2 \\
0 & 0 & \tilde{b}_3 & c_3 & \tilde{g}_3 \\
0 & 0 & a_4 & b_4 & g_4
\end{array}\right]
$$

- Last step

$R_4 \rightarrow R_4 - \frac{a_4}{\tilde{b}_3} R_3$

Define:
- $\tilde{b}_4 = b_4 - \frac{a_4}{\tilde{b}_3} c_3$
- $\tilde{g}_4 = g_4 - \frac{a_4}{\tilde{b}_3} \tilde{g}_3$

$$
\Rightarrow \left[\begin{array}{cccc|c}
\tilde{b}_1 & c_1 & 0 & 0 & \tilde{g}_1 \\
0 & \tilde{b}_2 & c_2 & 0 & \tilde{g}_2 \\
0 & 0 & \tilde{b}_3 & c_3 & \tilde{g}_3 \\
0 & 0 & 0 & \tilde{b}_4 & \tilde{g}_4
\end{array}\right]
$$

<u>Forward subst. done!</u>

For coding: No need for matrix, but arrays for $\bar{a}, \bar{b}, \bar{c}, \bar{g}, \bar{\tilde{b}}, \bar{\tilde{g}}, \bar{v}$

Forward subst. :

$$\left[\begin{array}{ll} \tilde{b}_1 = b_1 & \\ \tilde{b}_i = b_i - \dfrac{a_i}{\tilde{b}_{i-1}} c_{i-1} & , \text{for } i = 2,3,4 \\ & \\ \tilde{g}_1 = g_1 & \\ \tilde{g}_i = g_i - \dfrac{a_i}{\tilde{b}_{i-1}} \tilde{g}_{i-1} & \text{for } i = 2,3,4 \end{array}\right]$$

→ ◦ Back subst.

Starting point:

$$\begin{bmatrix} \tilde{b}_1 & c_1 & 0 & 0 \\ 0 & \tilde{b}_2 & c_2 & 0 \\ 0 & 0 & \tilde{b}_3 & c_3 \\ 0 & 0 & 0 & \tilde{b}_4 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} \tilde{g}_1 \\ \tilde{g}_2 \\ \tilde{g}_3 \\ \tilde{g}_4 \end{bmatrix} \Rightarrow \tilde{b}_4 v_4 = \tilde{g}_4$$

$$\Rightarrow \boxed{v_4 = \frac{\tilde{g}_4}{\tilde{b}_4}}$$

$$R_4 \to \frac{R_4}{\tilde{b}_4}$$

$$\left[\begin{array}{cccc|c} \tilde{b}_1 & c_1 & 0 & 0 & \tilde{g}_1 \\ 0 & \tilde{b}_2 & c_2 & 0 & \tilde{g}_2 \\ 0 & 0 & \tilde{b}_3 & c_3 & \tilde{g}_3 \\ 0 & 0 & 0 & 1 & v_4 \end{array}\right] \quad \left(= \frac{\tilde{g}_4}{\tilde{b}_4}\right)$$

$$R_3 \to (R_3 - c_3 R_4) / \tilde{b}_3$$

$$\begin{array}{ccccl} \tilde{b}_1 & c_1 & 0 & 0 & \tilde{g}_1 \\ 0 & \tilde{b}_2 & c_2 & 0 & \tilde{g}_2 \\ 0 & 0 & 1 & 0 & (\tilde{g}_3 - c_3 v_4)/\tilde{b}_3 = v_3 \quad ! \\ 0 & 0 & 0 & 1 & v_4 \end{array}$$

$$\Rightarrow \quad V_3 = \frac{\tilde{g}_3 - c_3 V_4}{\tilde{b}_3}$$

- Can continue upwards like this. In the end

$$\left[\begin{array}{ll} V_4 = \dfrac{\tilde{g}_4}{\tilde{b}_4} & \\ & \\ V_i = \dfrac{\tilde{g}_i - c_i V_{i+1}}{\tilde{b}_i} & i = 3, 2, 1 \end{array} \right]$$

Back subst. done!

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & 0 & v_1 \\ 0 & 1 & 0 & 0 & v_2 \\ 0 & 0 & 1 & 0 & v_3 \\ 0 & 0 & 0 & 1 & v_4 \end{array}\right]$$

- Using Gaussian elim. on a general tridiag matrix (4×4) we have solved

$$A \bar{v} = \bar{g}$$

for $\bar{v} = [v_1, v_2, v_3, v_4]$

Two parts to procedure:

- Forward subst. / elim.
- Back subst.

- Possible question: Why do all this stuff? Why not rather find A^{-1} and say

$$\bar{v} = A^{-1} \bar{g} \ ?$$

Answer: Finding A^{-1} takes $\mathcal{O}(n^3)$ operations. Useful if solving <u>many</u> eqs. with A; but for only a single eq. $A\bar{v} = \bar{g}$, other methods are quicker.

$$A \bar{v}_1 = \bar{g}_1$$
$$A \bar{v}_2 = \bar{g}_2$$
$$A \bar{v}_3 = \bar{g}_3$$
$$\vdots$$