Recap:

- Introduced notation for discretization: $x \to x_i$ $\quad x_0, x_1, \dots, x_n$
  $u(x) \to u_i$ $\quad u_0, u_1, \dots, u_n$

- Derivatives

$$\left.\frac{du}{dx}\right|_{x_i} = u_i' = \begin{cases} \dfrac{u_{i+1} - u_i}{h} + \mathcal{O}(h) \\ \dfrac{u_i - u_{i-1}}{h} + \mathcal{O}(h) \\ \dfrac{u_{i+1} - u_{i-1}}{2h} + \mathcal{O}(h^2) \end{cases}$$

$$\left.\frac{d^2u}{dx^2}\right|_{x_i} = u''_i = \frac{u_{i+1} - 2u + u_{i-1}}{h^2} + \mathcal{O}(h^2)$$

[Good news and bad news:
– Bad: Lot's of tedious writing
– Good: Will help you a lot with Proj. 1]

Next:

- Boundary value problem (example in Pr. 1)
- Formulation as a matrix problem
- Solving matrix eqs., with special focus on tridiag. matrices
- Floating point operations (FLOPs)
- Errors

Background material: Sec 6.4 (6.4.5)

Note: Differences in notation!
Also, some index typos, I think...

Boundary value problem

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

- Special case of :

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

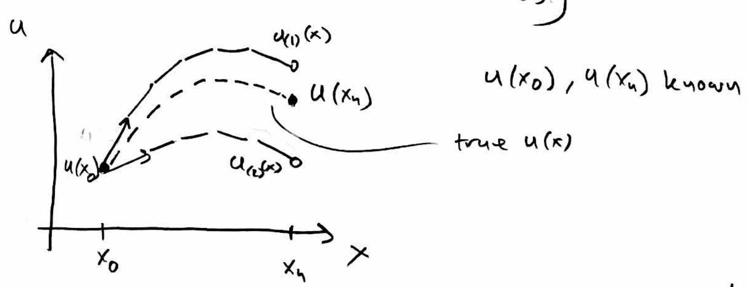
- Ordinary diff. eq. (only one indep. variable x)
- Linear diff. eq. (each term has max. one power of $u, u', u'', \ldots$)
- Second order (highest-order derivative is u'')
- Inhomogeneous ($f(x) \neq 0$)

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

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

Most famous example
Schr. eq. in QM is linear
↳ Superposition of quantum states!

- Shooting method intuition
    - Turn BVP 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

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

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

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

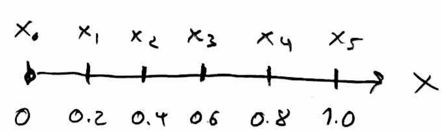
- Arrange terms

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

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

- Here: $n = 5$ steps
  $v_0, v_1, v_2, v_3, v_4, v_5$: 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!

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

- v_0, v_5 are known

define notation ↓

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

- 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 general matrix eq. $A\bar{v} = \bar{g}$

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

  Now → 2) Solving $A\bar{v} = \bar{g}$ when A is a general tridiagonal matrix

     Gauss elim. ⇒ Thomas algorithm

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

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

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

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

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 $m = n \Leftrightarrow A$ is square
  $\Leftrightarrow$ 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 → no exact solution, but can fit unknowns. Typical case in science!]

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

- **Gaussian elimination**

$$\begin{array}{ccccc} A & \bar{v} & = & \bar{g} \end{array}$$

$$\begin{bmatrix} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \end{bmatrix} \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix} = \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix}$$

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

$$\begin{bmatrix} \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet \\ & 0 & \bullet & \bullet \\ & & & \bullet \end{bmatrix} \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix} = \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix}$$

upper triangular

trivial to solve for last v_i

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

$$\begin{bmatrix} 1 & & & \\ & 1 & 0 & \\ & 0 & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix} = \begin{bmatrix} \bullet \\ \bullet \\ \bullet \\ \bullet \end{bmatrix}$$

solved for all v_i

- Our case : <u>General tridiagonal A</u>

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

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

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

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

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

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

- 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: $R_3 \to R_3 - \frac{a_3}{b_2} R_2$

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

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

- Last step

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

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

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

Forward subst. done!

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:

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

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

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

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

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

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

$$\Rightarrow \quad v_3 = \frac{\tilde{g}_3 - c_3 v_4}{\tilde{b}_3}$$

- Can continue upwards like this. In the end

$$\left[\begin{aligned} v_4 &= \frac{\tilde{g}_4}{\tilde{b}_4} \\ v_i &= \frac{\tilde{g}_i - c_i v_{i+1}}{\tilde{b}_i} \qquad i = 3, 2, 1 \end{aligned}\right]$$

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.