Application: finite differences

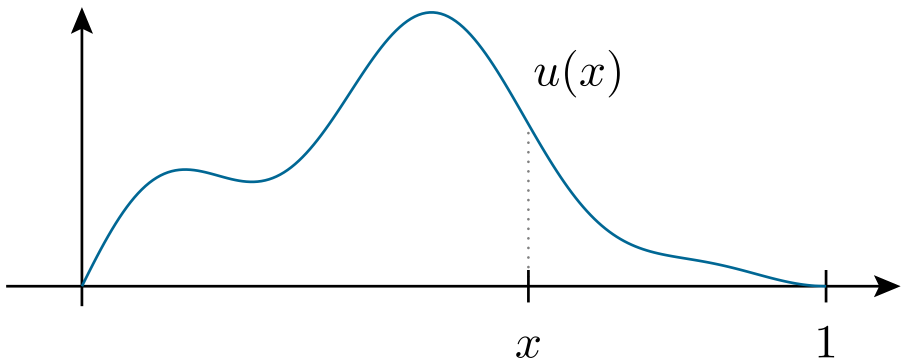
Let us apply linear algebra to the **boundary value problem**

$$-\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = f(x), \quad 0 \leqslant x \leqslant 1, \qquad u(0) = u(1) = 0.$$

$f(x)$ is given, and the goal is to find $u(x)$.

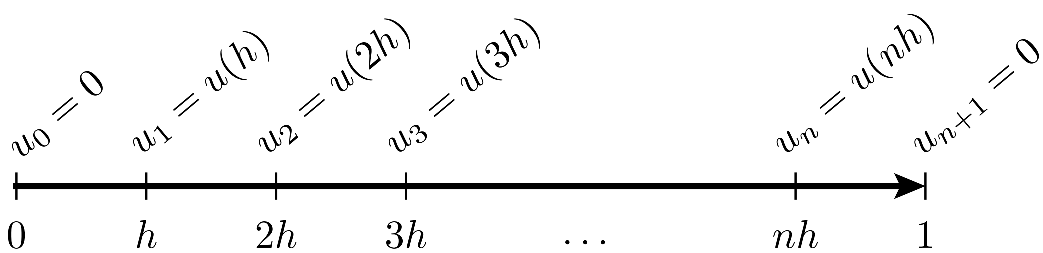
Physical interpretation: models steady-state temperature distribution in a bar ($u(x)$ is temperature at point x) under influence of an external heat source $f(x)$ and with ends fixed at $0°$ (ice cube at the ends?).

The boundary condition $u(0) = u(1) = 0$ makes the solution $u(x)$ unique.



We will approximate this problem as follows:

- replace $u(x)$ by its values at equally spaced points in $[0,1]$



- approximate $\frac{\mathrm{d}^2u}{\mathrm{d}x^2}$ at these points (**finite differences**)
- replace differential equation with linear equation at each point
- solve linear problem using Gaussian elimination

Finite differences

Finite differences for first derivative:

$$\frac{\mathrm{d}u}{\mathrm{d}x} \approx \frac{\Delta u}{\Delta x} = \frac{u(x+h) - u(x)}{h} \overset{\text{or}}{=} \frac{u(x) - u(x-h)}{h} \overset{\text{or}}{=} \frac{u(x+h) - u(x-h)}{2h}$$

symmetric and most accurate

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Finite differences for second derivative:

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

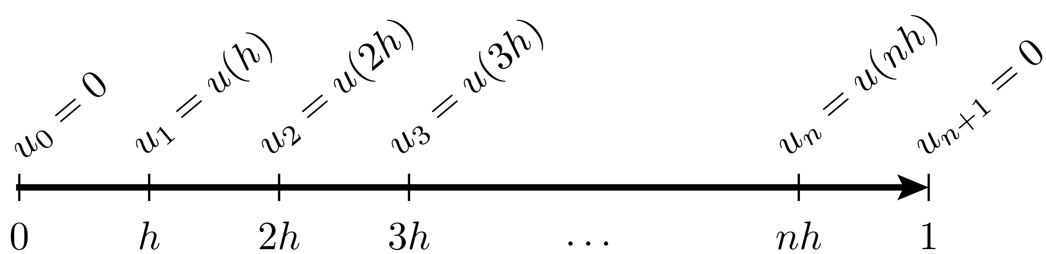
the only symmetric choice involving only $u(x)$, $u(x \pm h)$

Question 1. Why does this approximate $\frac{\mathrm{d}^2u}{\mathrm{d}x^2}$ as $h \to 0$?

Setting up the linear equations

$$-\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = f(x), \quad 0 \leqslant x \leqslant 1, \qquad u(0) = u(1) = 0.$$

Using $\frac{\mathrm{d}^2u}{\mathrm{d}x^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$, we get:



at $x = h$: $\quad -\frac{u(2h) - 2u(h) + u(0)}{h^2} = f(h)$

$\Longrightarrow \quad 2u_1 - u_2 = h^2 f(h) \qquad (1)$

at $x = 2h$:

$\Longrightarrow \qquad (2)$

at $x = 3h$:

$\Longrightarrow \qquad (3)$

$\vdots$

at $x = nh$:

$\Longrightarrow \qquad (n)$

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Example 2. In the case of six divisions ($n = 5$), we get:

$$\underbrace{\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}}_{\boldsymbol{x}} = \underbrace{\begin{bmatrix} h^2 f(h) \\ h^2 f(2h) \\ h^2 f(3h) \\ h^2 f(4h) \\ h^2 f(5h) \end{bmatrix}}_{\boldsymbol{b}}$$

Such a matrix is called a **band matrix**. As we will see next, such matrices always have a particularly simple LU decomposition

Gaussian elimination:

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This leads to the LU decomposition:

Now, given an f, we can solve for $u_1, \ldots, u_5$ by forward and back substitution.

$$A\boldsymbol{x} = \boldsymbol{b} \quad \overset{A=LU}{\Longleftrightarrow} \quad L\boldsymbol{c} = \boldsymbol{b} \quad \text{and} \quad U\boldsymbol{x} = \boldsymbol{c}$$

LU decomposition vs matrix inverse

In many applications, we don't just solve $A\boldsymbol{x} = \boldsymbol{b}$ for a single $\boldsymbol{b}$, but for many different $\boldsymbol{b}$ (think millions).

Note, for instance, that in our example of "steady-state temperature distribution in a bar" the matrix A is always the same (it only depends on the kind of problem), whereas the vector $\boldsymbol{b}$ models the external heat (and thus changes for each specific instance).

- That's why the LU decomposition saves us from repeating lots of computation in comparison with Gaussian elimination.
- What about computing A^{-1}? [Not just here, using A^{-1} is a bad idea!]

Example 3. Using LU decomposition, we solve, for each $\boldsymbol{b}$,

$$\begin{bmatrix} 1 & & & & \\ -\frac{1}{2} & 1 & & & \\ & -\frac{2}{3} & 1 & & \\ & & -\frac{3}{4} & 1 & \\ & & & -\frac{4}{5} & 1 \end{bmatrix} \boldsymbol{c} = \boldsymbol{b}, \quad \begin{bmatrix} 2 & -1 & & & \\ & \frac{3}{2} & -1 & & \\ & & \frac{4}{3} & -1 & \\ & & & \frac{5}{4} & -1 \\ & & & & \frac{6}{5} \end{bmatrix} \boldsymbol{x} = \boldsymbol{c}$$

by forward and backward substitution.

How many operations are needed in the $n \times n$ case?

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On the other hand,

$$A^{-1} = \frac{1}{6}\begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ 4 & 8 & 6 & 4 & 2 \\ 3 & 6 & 9 & 6 & 3 \\ 2 & 4 & 6 & 8 & 4 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix}.$$

How many operations are needed to compute $A^{-1}\boldsymbol{b}$?

Conclusions

- Large matrices met in applications usually are not random but have some structure (such as band matrices).
- When solving linear equations, we do not (try to) compute A^{-1}.
  - It destroys structure in practical problems.
  - As a result, it can be orders of magnitude slower,
  - and require orders of magnitude more memory.
  - It is also numerically unstable.
  - LU decomposition can be adjusted to not have these drawbacks.

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