TW4014TU – Numerical Analysis for PDE's

Lecture 3
Finite Difference Method in 1D, order of approximation, properties of 1D FD Laplacian

Finite-Difference Method in 1D

1D problem

We want to solve a 1D boundary value problem for the Poisson equation with Dirichlet BC's and different source functions:

$$-\frac{d^2u}{dx^2} = f, \quad x \in (0,1)$$

$$u(0) = 0, \quad u(1) = 0$$

case 1: $f(x) = -1$

case 2: $f(x) = -x + x^2 - x^3 + x^4 - x^5 + x^6$

case 3: $f(x) = -\sin(\pi x)$

Analytical solutions

This is an ordinary linear second-order differential equation, which can be solved analytically:

case 1: $f(x) = -1$;

$$u = -\frac{1}{2}x + \frac{1}{2}x^2$$

case 2: $f(x) = -x + x^2 - x^3 + x^4 - x^5 + x^6$;

$$u = -\frac{1}{840}(15x^8 - 20x^7 + 28x^6 - 42x^5 + 70x^4 - 140x^3 + 89x)$$

case 3: $f(x) = -\sin(\pi x)$;

$$u = -\frac{1}{\pi^2}\sin(\pi x)$$

1D Grid

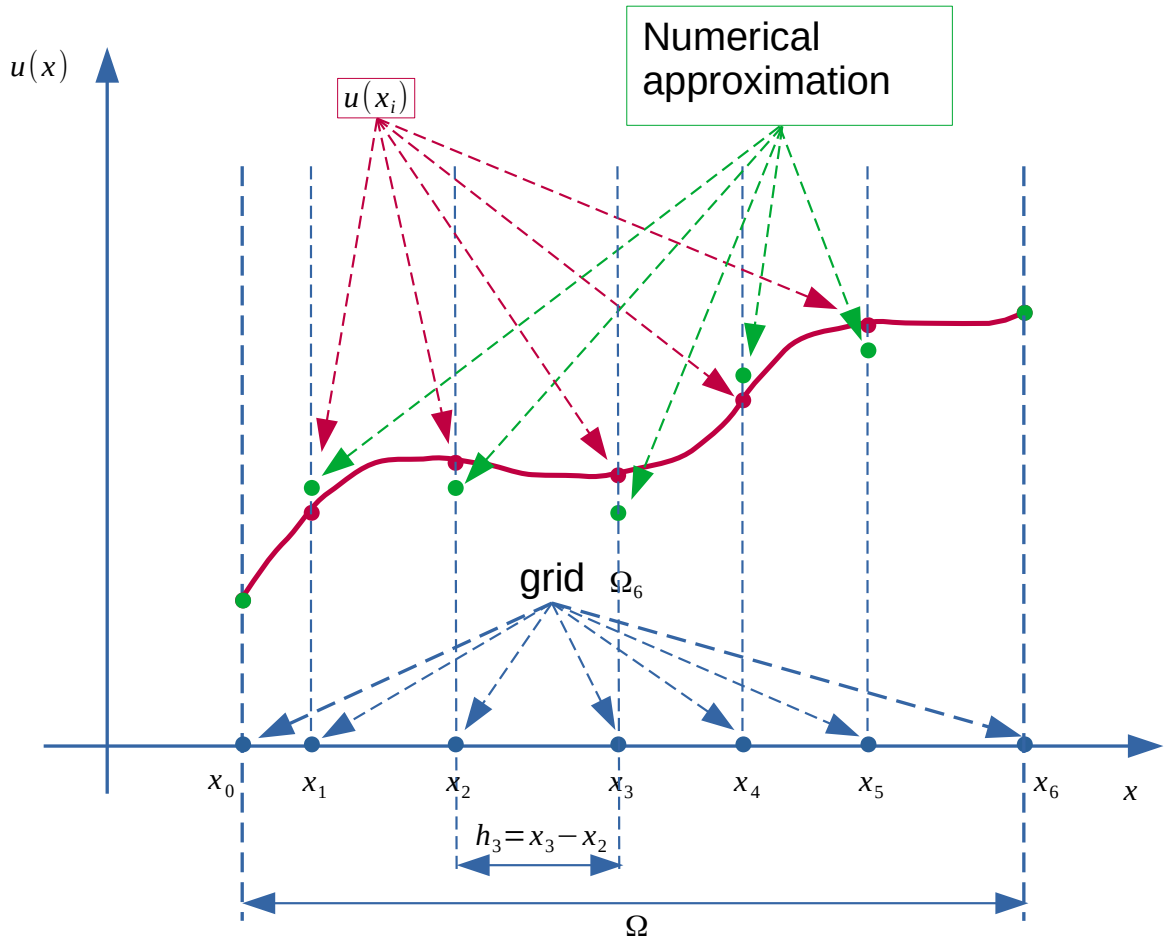
- A **grid** (mesh) on a segment $\Omega = [a, b]$ is any finite set of points of this segment. We denote as Ω_N the grid satisfying the following property:

$$a = x_0 < x_1 < x_2 < \cdots < x_{N-1} < x_N = b$$

  These are the boundaries of the N sub-intervals dividing the domain Ω.

- Points x_i are called the **nodes** of the grid Ω_N
- We denote as f_i the **grid value** of the function $f(x)$ at the point $x_i \in \Omega_N$, i.e., $f_i = f(x_i)$ or $u_i = u(x_i)$.
- **Inner points/nodes**: x_i, $i = 1, \ldots, N-1$. **Boundary points/nodes** x_0 and x_N.

Idea of numerical solution



Equation at grid nodes

Let $u(x)$ be a sufficiently smooth function defined on Ω. Introducing Ω_h on Ω, $f_i = f(x_i)$ and $u_i = u(x_i)$ we write the PDE at x_i:

$$-u_i'' = f_i, \quad i = 1, 2, \ldots, N-1,$$

and the two boundary conditions

$$u_0 = 0, \quad u_N = 0.$$

Here f_i, u_0, and u_N are known. Unknowns are the values of u_i, $i = 1, \ldots, N-1$; at the internal grid points x_i, $i = 1, \ldots, N-1$.

We need a connection between the derivative u_i'' at x_i and the grid values u_i, $i = 0, \ldots, N$. First we study the connection proposed by the Finite-Difference Method.

Deriving a Finite-Difference formula for $-u_i''$

Taylor series of $u(x)$ around x_i:

$$u(x) = u(x_i) + u'(x_i)(x - x_i) + \frac{u''(x_i)}{2}(x - x_i)^2 + \frac{u'''(x_i)}{6}(x - x_i)^3 + \ldots$$
$$= u_i + u_i'(x - x_i) + \frac{u_i''}{2}(x - x_i)^2 + \frac{u_i'''}{6}(x - x_i)^3 + \ldots$$

Take the nodes x_{i+1} and x_{i-1}:

$$u_{i+1} = u_i + u_i'(x_{i+1} - x_i) + \frac{u_i''}{2}(x_{i+1} - x_i)^2 + \frac{u_i'''}{6}(x_{i+1} - x_i)^3 + \ldots$$
$$u_{i-1} = u_i + u_i'(x_{i-1} - x_i) + \frac{u_i''}{2}(x_{i-1} - x_i)^2 + \frac{u_i'''}{6}(x_{i-1} - x_i)^3 + \ldots$$

Deriving a Finite-Difference formula for $-u_i''$

Rearrange:

$$-\frac{u_i''}{2}(x_{i+1}-x_i)^2 = -u_{i+1}+u_i+u_i'(x_{i+1}-x_i)+\frac{u_i'''}{6}(x_{i+1}-x_i)^3+\ldots$$
$$-\frac{u_i''}{2}(x_{i-1}-x_i)^2 = -u_{i-1}+u_i+u_i'(x_{i-1}-x_i)+\frac{u_i'''}{6}(x_{i-1}-x_i)^3+\ldots$$

Divide:

$$-\frac{u_i''}{2} = \frac{-u_{i+1}+u_i}{(x_{i+1}-x_i)^2}+u_i'\frac{x_{i+1}-x_i}{(x_{i+1}-x_i)^2}+\frac{u_i'''}{6}\frac{(x_{i+1}-x_i)^3}{(x_{i+1}-x_i)^2}+\ldots$$
$$-\frac{u_i''}{2} = \frac{-u_{i-1}+u_i}{(x_{i-1}-x_i)^2}+u_i'\frac{x_{i-1}-x_i}{(x_{i-1}-x_i)^2}+\frac{u_i'''}{6}\frac{(x_{i-1}-x_i)^3}{(x_{i-1}-x_i)^2}+\ldots$$

Deriving a Finite-Difference formula for $-u_i''$

Simplify:

$$-\frac{u_i''}{2} = \frac{-u_{i+1} + u_i}{(x_{i+1} - x_i)^2} + u_i' \frac{1}{x_{i+1} - x_i} + \frac{u_i'''}{6}(x_{i+1} - x_i) + \ldots$$
$$-\frac{u_i''}{2} = \frac{-u_{i-1} + u_i}{(x_{i-1} - x_i)^2} + u_i' \frac{1}{x_{i-1} - x_i} + \frac{u_i'''}{6}(x_{i-1} - x_i) + \ldots$$

Add:

$$\begin{aligned} -u_i'' = & \frac{-u_{i+1} + u_i}{(x_{i+1} - x_i)^2} + \frac{-u_{i-1} + u_i}{(x_{i-1} - x_i)^2} \\ & + u_i' \frac{1}{x_{i+1} - x_i} + u_i' \frac{1}{x_{i-1} - x_i} \\ & + \frac{u_i'''}{6}(x_{i+1} - x_i) + \frac{u_i'''}{6}(x_{i-1} - x_i) + \ldots \end{aligned}$$

Finite-Difference approximation of $-u_i''$ on a uniform grid

Uniform grid: $x_{i+1} - x_i = h$, $i = 0, \ldots, N$. Note that $x_{i-1} - x_i = -h$.

$$
\begin{aligned}
-u_i'' = & \frac{-u_{i+1} + u_i}{h^2} + \frac{-u_{i-1} + u_i}{h^2} \\
& + u_i' \frac{1}{h} - u_i' \frac{1}{h} + \frac{u_i'''}{6} h - \frac{u_i'''}{6} h + \\
& + \frac{u_i^{(4)}}{24} h^2 + \frac{u_i^{(4)}}{24} h^2 + \ldots
\end{aligned}
$$

Hence,

$$
-u_i'' = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} + \frac{u_i^{(4)}}{12} h^2 + \ldots
$$

Order of approximation

$$-u_i'' = \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} + \mathcal{O}(h^2)$$

Here, $\mathcal{O}(h^2)$ is the **order of approximation**. It is the local approximation error:

$$\text{local approx. error} = \left| -u_i'' - \frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} \right| = \mathcal{O}(h^2)$$

This "central difference" formula is order-h^2 (second-order) approximation of $-u''$ at x_i, if the grid is uniform.
If we define the central-difference FD approximation of u_i'' as:

$$\mathcal{D}_{xx}^{(2)} u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2},$$

then $\left| u_i'' - \mathcal{D}_{xx}^{(2)} u_i \right| = \mathcal{O}(h^2)$

Finite-Difference approximations for u_i'

- The **left finite-difference derivative** (one-sided, backward)

$$\mathcal{D}_x^- u_i = \frac{u_i - u_{i-1}}{h}$$

- The **right finite-difference derivative** (one-sided, forward)

$$\mathcal{D}_x^+ u_i = \frac{u_{i+1} - u_i}{h}$$

- The **central finite-difference derivative** (two-sided)

$$\mathcal{D}_x^c u_i = \frac{u_{i+1} - u_{i-1}}{2h}$$

Derivation and order of $\mathcal{D}_x^- u_i$

Taylor series of $u(x)$ around x_i:

$$u(x) = u(x_i) + u'(x_i)(x - x_i) + \frac{u''(x_i)}{2}(x - x_i)^2 + \frac{u'''(x_i)}{6}(x - x_i)^3 + \dots$$
$$= u_i + u_i'(x - x_i) + \frac{u_i''}{2}(x - x_i)^2 + \frac{u_i'''}{6}(x - x_i)^3 + \dots$$

Take the node x_{i-1}:

$$u_{i-1} = u_i + u_i'(x_{i-1} - x_i) + \frac{u_i''}{2}(x_{i-1} - x_i)^2 + \frac{u_i'''}{6}(x_{i-1} - x_i)^3 + \dots$$
$$-u_i'(x_{i-1} - x_i) = -u_{i-1} + u_i + \frac{u_i''}{2}(x_{i-1} - x_i)^2 + \frac{u_i'''}{6}(x_{i-1} - x_i)^3 + \dots$$
$$-u_i' = \frac{-u_{i-1} + u_i}{x_{i-1} - x_i} + \frac{u_i''}{2}(x_{i-1} - x_i) + \frac{u_i'''}{6}(x_{i-1} - x_i)^2 + \dots$$
$$u_i' = \frac{u_i - u_{i-1}}{h} + \mathcal{O}(h)$$

Derivation and order of $\mathcal{D}_x^+ u_i$

Take the node x_{i+1}:

$$u_{i+1} = u_i + u_i'(x_{i+1} - x_i) + \frac{u_i''}{2}(x_{i+1} - x_i)^2 + \frac{u_i'''}{6}(x_{i+1} - x_i)^3 + \ldots$$

$$-u_i'(x_{i+1} - x_i) = -u_{i+1} + u_i + \frac{u_i''}{2}(x_{i+1} - x_i)^2 + \frac{u_i'''}{6}(x_{i+1} - x_i)^3 + \ldots$$

$$-u_i' = \frac{-u_{i+1} + u_i}{x_{i+1} - x_i} + \frac{u_i''}{2}(x_{i+1} - x_i) + \frac{u_i'''}{6}(x_{i+1} - x_i)^2 + \ldots$$

$$u_i' = \frac{u_{i+1} - u_i}{h} + \mathcal{O}(h)$$

Derivation and order of $\mathcal{D}_x^c u_i$ on a uniform grid

Take the nodes x_{i-1} and x_{i+1}:

$$u_{i-1} = u_i - u_i' h + \frac{u_i''}{2} h^2 - \frac{u_i'''}{6} h^3 + \ldots$$

$$u_{i+1} = u_i + u_i' h + \frac{u_i''}{2} h^2 + \frac{u_i'''}{6} h^3 + \ldots$$

$$u_i' h = -u_{i-1} + u_i + \frac{u_i''}{2} h^2 - \frac{u_i'''}{6} h^3 + \ldots$$

$$u_i' h = u_{i+1} - u_i - \frac{u_i''}{2} h^2 - \frac{u_i'''}{6} h^3 + \ldots$$

$$2u_i' h = -u_{i-1} + u_{i+1} - \frac{u_i'''}{3} h^3 + \ldots$$

$$u_i' = \frac{u_{i+1} - u_{i-1}}{2h} - \frac{u_i'''}{6} h^2 + \ldots$$

$$u_i' = \frac{u_{i+1} - u_i}{2h} + \mathcal{O}(h^2)$$

Connection between FD approximations of u' and u''

On a uniform grid the second FD derivative can be written via the first one-sided FD derivatives as:

$$\mathcal{D}^{(2)}_{xx} u_i = \frac{\mathcal{D}^{+}_{x} u_i - \mathcal{D}^{-}_{x} u_i}{h} = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

FD method in a nutshell

Continuous problem:

$$
\begin{aligned}
-\frac{\partial^2 u}{\partial x^2} &= f, \quad x \in (0,1) \\
u(0) &= 0, \quad u(1) = 0 \\
\text{case 1:} \quad f(x) &= -1 \\
\text{case 2:} \quad f(x) &= -x + x^2 - x^3 + x^4 - x^5 + x^6 \\
\text{case 3:} \quad f(x) &= -\sin(\pi x_i)
\end{aligned}
$$

FD method: choose $h = 1/N$, define Ω_h on $[0,1]$, solve

$$
\begin{aligned}
-\mathcal{D}_{xx}^{(2)} u_i &= f_i, \quad x_i \in \omega_h \\
u_0 &= 0, \quad u_N = 0 \\
\text{case 1:} \quad f_i &= -1 \\
\text{case 2:} \quad f_i &= -x_i + x_i^2 - x_i^3 + x_i^4 - x_i^5 + x_i^6 \\
\text{case 3:} \quad f_i &= -\sin(\pi x_i)
\end{aligned}
$$

FD method vs analytical solutions

- Since $\mathcal{D}_{xx}^{(2)} u_i$ is an approximation of $u''(x_i)$, the numerical solution of a differential equation obtained by the FD method will be an *approximation* of $u(x_i)$, $i = 1, \ldots, N-1$.
- If we know the analytical solution of the problem, then we can *compute* the error of the FD method (Assignment 2)
- In general we do not know the analytical solution, but we can still *estimate* the error of the FD method (next Lecture)

FDM Step 1: write discrete FD equations

Continuous problem:

$$-u'' = f, \quad x \in \Omega = (a, b);$$
$$u(a) = g_0, \quad u(b) = g_1$$

Discrete FD equations:

$$u_0 = g_0 \quad \text{left BC}$$
$$-\frac{1}{h^2}(u_0 - 2u_1 + u_2) = f_1$$
$$-\frac{1}{h^2}(u_1 - 2u_2 + u_3) = f_2$$
$$\dots$$
$$-\frac{1}{h^2}(u_{N-2} - 2u_{N-1} + u_N) = f_{N-1}$$
$$u_N = g_1 \quad \text{right BC}$$

FDM Step 2: eliminate u_0 and u_N

Boundary values u_0 and u_N are usually eliminated and the BC's are shifted to the right-hand side:

$$
\begin{aligned}
-\frac{1}{h^2}(-2u_1 + u_2) &= f_1 + \frac{1}{h^2}g_0 \\
-\frac{1}{h^2}(u_1 - 2u_2 + u_3) &= f_2 \\
&\dots \\
-\frac{1}{h^2}(u_{N-2} - 2u_{N-1}) &= f_{N-1} + \frac{1}{h^2}g_1
\end{aligned}
$$

FDM Step 3: Assemble system matrix and RHS vector

$$-\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ . & & & & & . \\ . & & & & & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 + g_0/h^2 \\ f_2 \\ . \\ . \\ f_{N-1} + g_1/h^2 \end{bmatrix}$$

Notice that the system matrix does not depend on g_0 and g_1.

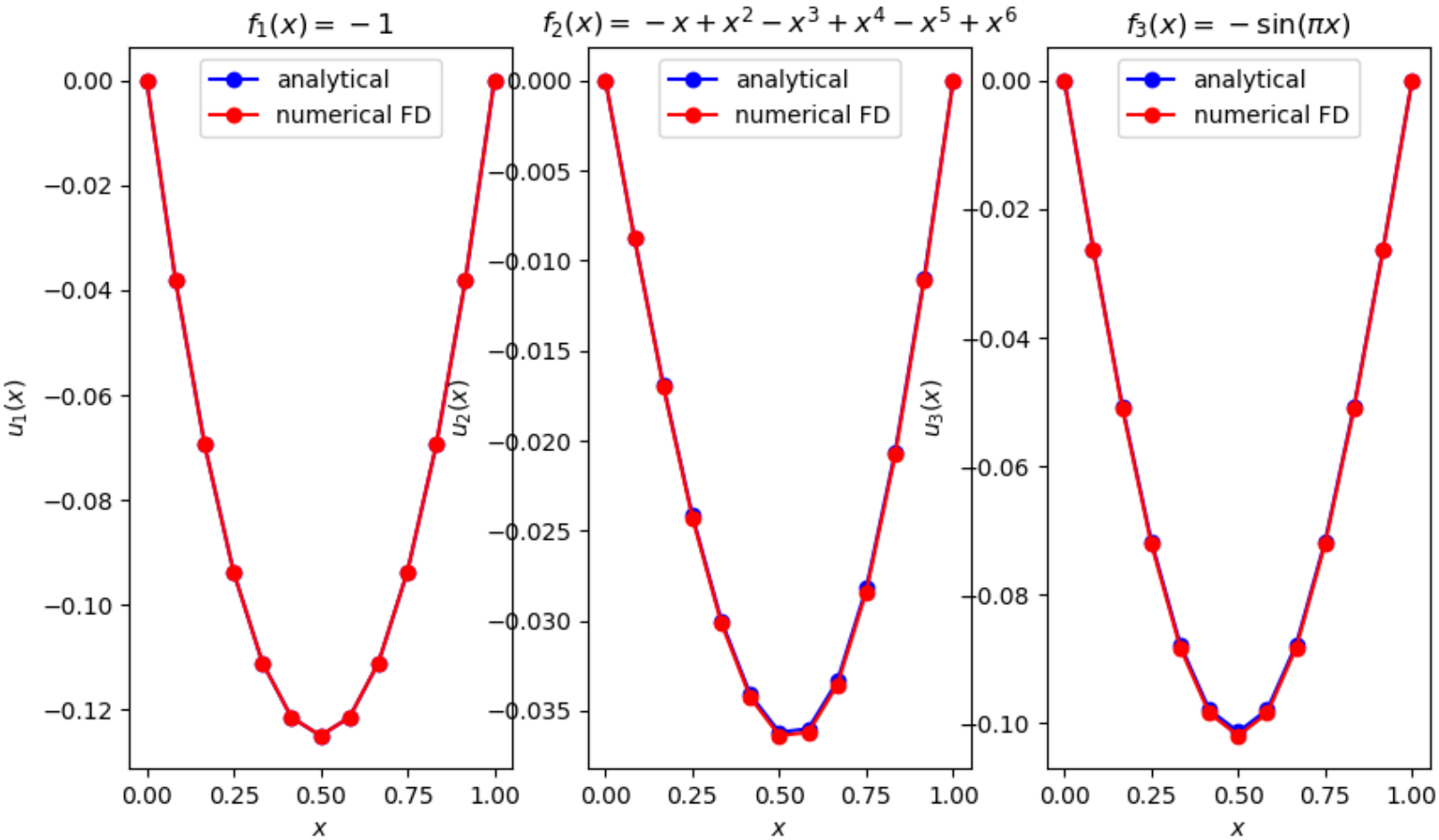
FDM Step 4: Solve linear algebraic problem

In matrix notation:

$$A\boldsymbol{u} = \boldsymbol{f}$$
$$\boldsymbol{u} = A^{-1}\boldsymbol{f}$$

The resulting vector $\boldsymbol{u} \in \mathbb{R}^{N-1}$ contains the FDM approximation of the grid-values of the solution $u(x_i)$ at the inner points of the grid $i = 1, \ldots, N-1$.

Matplotlib figures



Analysis of discretized PDE's

- For the continuous boundary-value problem

$$-\Delta u = f, \quad \boldsymbol{x} \in \Omega,$$
$$u = g, \quad \boldsymbol{x} \in \partial\Omega,$$

  we had the Maximum Principle and established that

  1. Solution $u(\boldsymbol{x})$ is unique
  2. Sometimes we can tell where the maximum/minimum is and whether $u(\boldsymbol{x})$ is positive/negative/constant

- After discretization with the Finite-Difference Method we arrived at the linear algebraic problem:

$$L\boldsymbol{u} = \boldsymbol{f}$$

  1. Does it have a unique solution?
  2. Can we say something about $\boldsymbol{u}$?
  3. How big is the error between the numerical u_i and the exact u_i?

Properties of 1D FD Laplacian

Central-difference 1D FD Laplacian matrix

Consider the matrix L corresponding to the central-difference FD approximation $-\mathcal{D}_{xx}^{(2)}$ of the negative Laplacian operator $-d^2/dx^2$ with Dirichlet BC's:

$$L = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ . & & & & & . \\ . & & & & & -1 \\ 0 & 0 & 0 & \dots & -1 & 2 \end{bmatrix}$$

What are the main properties?

Positive definiteness

Definition: Matrix $A \in \mathbb{R}^{n \times n}$ is *positive* if $\boldsymbol{u}^T A \boldsymbol{u} \geq 0$ and *positive definite* if $\boldsymbol{u}^T A \boldsymbol{u} > 0$ for all $\boldsymbol{u} \in \mathbb{R}^n$, $\boldsymbol{u} \neq 0$.

Theorem: The 1D FD (negative) Laplacian matrix L is *positive definite*.

Positive definiteness

Proof:

$$
\begin{aligned}
\boldsymbol{u}^T L\boldsymbol{u} &= \frac{1}{h^2}\left(2u_1^2 - u_1u_2 - u_1u_2 + 2u_2^2 - u_2u_3 + \cdots - u_{N-1}u_{N-2} + 2u_{N-1}^2\right) \\
&= \frac{1}{h^2}\left(u_1^2 + u_1^2 - 2u_1u_2 + u_2^2 + u_2^2 - 2u_2u_3 + u_3^2 + \right. \\
&\qquad \left. \cdots + u_{N-2}^2 - 2u_{N-1}u_{N-2} + u_{N-1}^2 + u_{N-1}^2\right) \\
&= \frac{1}{h^2}\left(u_1^2 + \sum_{i=1}^{N-2}(u_i - u_{i+1})^2 + u_{N-1}^2\right) > 0, \quad \text{if} \quad \boldsymbol{u} \neq 0
\end{aligned}
$$

Symmetry

Definition: A matrix $A \in \mathbb{R}^{n \times n}$ is *symmetric* if $A^T = A$.

Theorem: The 1D FD (negative) Laplacian matrix L is *symmetric positive definite* (an SPD matrix).

Corollaries:

1. There is an eigendecomposition $L = Q \Lambda Q^T$, where $Q^T Q = I$
2. All eigenvalues of L are distinct, real and positive. In particular, the smallest eigenvalue $\lambda_1 > 0$
3. The matrix L is invertible
4. There is a unique solution to the problem $L\boldsymbol{u} = \boldsymbol{f}$

Eigenvalues and eigenvectors

Let the grid step be $h = D/N$, where $D = x_N - x_0$ is the segment length. The eigenvalue problem is

$$L\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$$

The $N-1$ eigenvalues of the discrete FD Laplacian matrix $L \in \mathbb{R}^{(N-1)\times(N-1)}$ are given by:

$$\lambda_i = \frac{4}{h^2} \sin^2\left(\frac{\pi\, i}{2N}\right); \quad i = 1, 2, \ldots, N-1$$

The corresponding eigenvectors v_i of L have elements

$$[\boldsymbol{v}_i]_j = \sin\left(\frac{\pi\, i\, j}{N}\right); \quad i, j = 1, 2, \ldots, N-1$$

Correspondence with continuous problem

The eigenvalues and eigenfunctions of the original continuous problem $-v_i'' = \lambda_i v_i$, $v_i(0) = v_i(D) = 0$ are:

$$\tilde{\lambda}_i = \left(\frac{\pi\, i}{D}\right)^2, \quad v_i(x) = \sin\left(\frac{\pi\, i\, x}{D}\right), \quad i = 1, 2, \ldots$$

Hence, since $x_j = jh$ and $h = D/N$, the eigevectors of the FD Laplacian are the exact sampled eigefunctions of the continuous Laplacian:

$$[\boldsymbol{v}_i]_j = v_i(x_j)$$

Whereas, the eigenvalues λ_i of the matrix L tend to the eigenvalues $\tilde{\lambda}_i$ of the continuous Laplacian $-d^2/dx^2$ in the limit, as $h \to 0$:

$$\lim_{h\to 0} \frac{4}{h^2} \sin^2\left(\frac{\pi ih}{2D}\right) = \left(\frac{\pi i}{D}\right)^2, \quad i = 1, 2, \ldots, N-1$$

The smallest eigenvalue

The smallest eigenvalue of L is

$$\lambda_1 = \frac{4}{h^2} \sin^2\left(\frac{\pi}{2N}\right)$$

The smallest eigenvalue of $-d^2/dx^2$ is

$$\tilde{\lambda}_1 = \left(\frac{\pi}{D}\right)^2$$