Chapter 4: contents

- Finite difference approximation of derivatives
- Finite difference methods for the 2p-BVP
- Newton’s method
- Sturm–Liouville problems
- Toeplitz matrices
- Convergence: Lax’ equivalence theorem
- Differential operators
- From finite differences to finite elements
1. Approximation of derivatives \((y' = \frac{dy}{dx})\)

*First order approximations*

**Forward difference**

\[
y'(x) = \frac{y(x + \Delta x) - y(x)}{\Delta x} + O(\Delta x)
\]

**Backward difference**

\[
y'(x) = \frac{y(x) - y(x - \Delta x)}{\Delta x} + O(\Delta x)
\]
Approximation of derivatives . . .

Second order approximations

Symmetric difference quotients

\[ y'(x) = \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x} + O(\Delta x^2) \]

\[ y''(x) = \frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} + O(\Delta x^2) \]
Derivatives → finite differences → matrices

Matrix representation of *forward difference*

\[
y'(x) = \frac{y(x + \Delta x) - y(x)}{\Delta x} + O(\Delta x)
\]

Introduce vectors \( y = \{y(x_i)\} \) and \( y' = \{y'(x_i)\} \):

\[
\begin{pmatrix}
y'_0 \\
y'_1 \\
\vdots \\
y'_N
\end{pmatrix}
\approx \frac{1}{\Delta x}
\begin{pmatrix}
-1 & 1 \\
-1 & 1 \\
\vdots & \vdots \\
-1 & 1
\end{pmatrix}
\begin{pmatrix}
y_0 \\
y_1 \\
\vdots \\
y_{N+1}
\end{pmatrix}
\]
Derivatives . . . matrices

**Note**  Forward difference $\sim (N + 1) \times (N + 2)$ matrix

$$\begin{pmatrix}
y'_0 \\
y'_1 \\
\vdots \\
y'_N
\end{pmatrix} \approx \frac{1}{\Delta x}
\begin{pmatrix}
-1 & 1 & & & \\
-1 & 1 & & & \\
& \ddots & \ddots & & \\
& & -1 & 1 & \\
\end{pmatrix}
\begin{pmatrix}
y_0 \\
y_1 \\
\vdots \\
y_{N+1}
\end{pmatrix}$$

Nullspace spanned by $y = (1 \ 1 \ 1 \ldots 1)^T$

Compare nullspace of $d/dx : y = 1 \Rightarrow y' \equiv 0$

Analogous result for backward difference
Central difference

\[ y'(x) \approx \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x} \]

Matrix representation

\[
\begin{pmatrix}
  y'_1 \\
  y'_2 \\
  \vdots \\
  y'_{N + 1}
\end{pmatrix}
\approx
\frac{1}{2\Delta x}
\begin{pmatrix}
  -1 & 0 & 1 \\
  \cdots & \cdots & \cdots \\
  -1 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
  y_0 \\
  y_1 \\
  \vdots \\
  y_{N + 1}
\end{pmatrix}
\]
Derivatives . . . matrices

**Note** \( N \times (N + 2) \) matrix

\[
\begin{pmatrix}
  y'_1 \\
y'_2 \\
  \vdots \\
y'_N
\end{pmatrix} \approx \frac{1}{2\Delta x} \begin{pmatrix}
-1 & 0 & 1 \\
  & \ddots & \ddots & \ddots \\
  &  & -1 & 0 & 1
\end{pmatrix} \begin{pmatrix}
y_0 \\
y_1 \\
  \vdots \\
y_{N+1}
\end{pmatrix}
\]

**Nullspace is two-dimensional:**
\[
\bar{y} = (1 \ 1 \ 1 \ldots 1)^T \quad \text{and} \quad \tilde{y} = (1 \ -1 \ 1 \ -1 \ldots 1)^T
\]
Derivatives . . . matrices

“False” nullspace \( \tilde{y} = (1 \ -1 \ 1 \ -1 \ldots 1)^T \) does not converge to a \( C^1 \) function!

Compare difference equation \( y_{n+1} - y_{n-1} = 0 \), with characteristic equation

\[ z^2 - 1 = 0 \quad \Rightarrow \quad z = \pm 1 \]

and solutions \( \bar{y}_n = 1 \) and \( \tilde{y}_n = (-1)^n \)
2nd order derivatives → matrices

Central difference

\[ y''(x) \approx \frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} \]

\[
\begin{pmatrix}
  y''_1 \\
  y''_2 \\
  \vdots \\
  y''_N
\end{pmatrix}
\approx \frac{1}{\Delta x^2}
\begin{pmatrix}
  1 & -2 & 1 & & & \\
  & \ddots & \ddots & \ddots & & \\
  & & 1 & -2 & 1 & \\
\end{pmatrix}
\begin{pmatrix}
  y_0 \\
  y_1 \\
  \vdots \\
  y_{N+1}
\end{pmatrix}
\]

Note \( N \times (N + 2) \) matrix with nullspace \( \bar{y} = (1 \ 1 \ldots 1)^T \)
and \( \hat{y} = (0 \ 1 \ 2 \ 3 \ldots N + 1)^T \)
2nd order derivatives . . .

**Nullspace** of \( \frac{d^2}{dx^2} \):

\( y = 1 \) and \( y = x \) both have \( y'' \equiv 0 \)

Compare difference equation \( y_{n+1} - 2y_n + y_{n-1} = 0 \), with characteristic equation

\[
z^2 - 2z + 1 = 0 \quad \Rightarrow \quad z = 1, 1
\]

and solutions \( \bar{y}_n = 1 \) and \( \hat{y}_n = n \), respectively
Numerical differentiation

First and second derivatives of $y = \sin \pi x$

Data function $\sin(\pi x)$ and sampled points for $h=1/6$

First derivative, fwd diff (+), bwd diff (x), symmetric diff (o)

Second derivative, symmetric 2nd diff (o)
2. Finite difference methods for 2p-BVP

Consider simplest problem

\[ y'' = f(x, y) \]

\[ y(0) = \alpha; \quad y(1) = \beta \]

Introduce equidistant grid with \( \Delta x = 1/(N + 1) \)

**Discretization**

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = f(x_i, y_i) \]

\[ y_0 = \alpha; \quad y_{N+1} = \beta \]
Discrete 2pBVP

\[
\frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = f(x_i, y_i) \quad i = 1 : N
\]

\[y_0 = \alpha; \quad y_{N+1} = \beta\]

This is a (nonlinear) system of equations \( F(y) = 0 \) for the \( N \) unknowns \( y_1, y_2, \ldots, y_N \)

Solve \( F(y) = 0 \) using Newton’s method
Equation system $F(y) = 0$

$$F_1(y) = \frac{\alpha - 2y_1 + y_2}{\Delta x^2} - f(x_1, y_1)$$

$$F_i(y) = \frac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} - f(x_i, y_i)$$

$$F_N(y) = \frac{y_{N-1} - 2y_N + \beta}{\Delta x^2} - f(x_N, y_N)$$

**Note** how *boundary values* enter
Jacobian matrix

\[ F'(y) = \text{tridiag} \left( \frac{1}{\Delta x^2}, -\frac{2}{\Delta x^2} + \frac{\partial f}{\partial y_i}, \frac{1}{\Delta x^2} \right) \]

is tridiagonal, and

- Super- and subdiagonal elements \( \frac{1}{\Delta x^2} \)
- Diagonal elements \( -\frac{2}{\Delta x^2} - \frac{\partial f}{\partial y_i} \)
- Sparse \( LU \) decomposition runs in \( O(N) \) time
- Solution effort moderate even when \( N \) is large
3. Newton’s method (recap)

Let $y^{(k)}$ be an approximation to the root $y$

Taylor series expansion

$$0 = F(y) \approx F(y^{(k)}) + F'(y^{(k)}) \cdot (y - y^{(k)})$$

Define $y^{(k+1)}$ by

$$0 =: F(y^{(k)}) + F'(y^{(k)}) \cdot (y^{(k+1)} - y^{(k)})$$
Newton’s method for $F(y) = 0$

Newton iteration

1. Compute Jacobian $F'(y^{(k)}) = \{ \partial F_i / \partial y_j \}$
2. Factorize Jacobian matrix $F'(y^{(k)}) \rightarrow LU$
3. Solve linear system $LU \delta y^{(k)} = -F(y^{(k)})$
4. Update $y^{(k+1)} := y^{(k)} + \delta y^{(k)}$

*Newton’s method is quadratically convergent*
Quadratic convergence

Newton’s method converges if

1. $\| F'(y^{(k)})^{-1} \| \leq C'$
2. $\| F''(y^{(k)}) \| \leq C''$
3. $\| y^{(0)} - y \| < \varepsilon$ (close enough starting value)

Then convergence is quadratic

$$\| y^{(k+1)} - y \| \leq C \cdot \| y^{(k)} - y \|^2$$
Boundary Conditions come in many shapes

- **“Dirichlet”** boundary conditions
  \[ y(0) = \alpha \] straightforward to implement

- **“Neumann”** boundary conditions
  \[ y'(0) = \gamma \] requires special attention

- **“Robin”** conditions
  \[ y(0) + c \cdot y'(0) = \kappa \] requires same attention

for the method’s *convergence order* to be preserved
Neumann problem

Example

\[ y'' = f(x, y) \]

\[ y(0) = \alpha; \quad y'(1) = \beta \]

Equidistant grid, with \( x = 1 \) between grid points!

\[ x_N + \Delta x/2 = 1 = x_{N+1} - \Delta x/2 \]

\[ y'(1) = \beta \quad \rightarrow \quad \frac{y_{N+1} - y_N}{\Delta x} = \beta \]

\( \Rightarrow \) \( y_{N+1} := \beta \Delta x + y_N \) is of second order at \( x = 1 \)
Robin problem

Example

\[ y'' = f(x, y) \]

\[ y(0) = \alpha; \quad y(1) + c \cdot y'(1) = \kappa \]

Equidistant grid, with \( x = 1 \) between grid points!

\[ y(1) + c y'(1) = \kappa \quad \rightarrow \quad \frac{y_{N+1} + y_N}{2} + c \frac{y_{N+1} - y_N}{\Delta x} = \kappa \]

\[ \Rightarrow \quad y_{N+1} := \frac{(2c - \Delta x)y_N + 2\kappa \Delta x}{2c + \Delta x} \]
4. Sturm–Liouville eigenvalue problems

Diffusion problem

\[
\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( p(x) \frac{\partial u}{\partial x} \right) = 0 ; \quad y(a) = 0 , \quad y(b) = 0
\]

Separation of variables (one space dimension)

\[
u(t, x) := y(x) \cdot v(t) \quad \Rightarrow \quad \frac{\dot{v}}{v} = \frac{(p(x) y'(x))'}{y} =: \lambda
\]

Sturm–Liouville eigenvalue problem

\[
\frac{d}{dx} \left( p(x) \frac{dy}{dx} \right) - \lambda y = 0 ; \quad y(a) = 0 , \quad y(b) = 0
\]
Sturm–Liouville eigenvalue problem ...

Wave equation

\[ \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}; \quad y(a) = \ldots , \quad y(b) = \ldots \]

Express solution as \( u(t, x) = y(x) e^{i\omega t} \Rightarrow \)

\[ -\omega^2 y = c^2 y'' \]

Sturm–Liouville eigenvalue problem

\[ y'' = \lambda y \quad \text{with} \quad \lambda = -\omega^2 / c^2 \]
Sturm–Liouville eigenvalue problem...

Find eigenvalues $\lambda$ and eigenfunctions $y(x)$ with

$$\frac{d}{dx} \left( p(x) \frac{dy}{dx} \right) = \lambda y ; \quad y(a) = 0 , \ y(b) = 0$$

Discretization Matrix eigenvalue problem

$$T_{\Delta x} y = \lambda_{\Delta x} y$$

Note Analytic eigenvalue problem converts to algebraic!
Sturm–Liouville problem. Discretization

\[
p_{i-1/2}y_{i-1} - \left( p_{i-1/2} + p_{i+1/2} \right) y_i + p_{i+1/2}y_{i+1} = \Delta x^2 \lambda_{\Delta x} y_i
\]

\[
y_0 = y_{N+1} = 0
\]

Symmetric tridiagonal $N \times N$ eigenvalue problem

\[
T_{\Delta x} y = \lambda_{\Delta x} y
\]

There are $N$ eigenvalues $\lambda_{\Delta x,n} = \lambda_n + O(\Delta x^2)$
Sturm–Liouville problem. Simple example

Example

\[ y'' = \lambda y \]
\[ y(0) = y(1) = 0 \]

Analytic solution

\[ y(x) = A \sin \sqrt{-\lambda} x + B \cos \sqrt{-\lambda} x \]

Boundary values \( \Rightarrow \) \( B = 0 \) and

\[ A \sin \sqrt{-\lambda} = 0 \]

\[ A \neq 0 \quad \Rightarrow \quad \sqrt{-\lambda} = n\pi \quad n = 1, 2, \ldots \]
Simple Sturm–Liouville example . . .

\[ y'' = \lambda y \]
\[ y(0) = y(1) = 0 \]

**Eigenvalues**  \[ \lambda_n = -n^2 \pi^2, \quad n = 1, 2, \ldots \]

**Eigenfunctions**  \[ y_n(x) = \sin n\pi x \]
Discrete Sturm–Liouville. Same example

**Discretization** of $y'' = \lambda y$ with BVs $\Rightarrow$

$$\frac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} = \lambda \Delta x y_i$$

$y_0 = y_{N+1} = 0$; $\Delta x = 1/(N + 1)$

Tridiagonal $N \times N$ matrix formulation

$$\frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 \\ 1 & -2 & 1 \\ & \ddots & \ddots \\ 1 & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \lambda \Delta x \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$
Discrete Sturm–Liouville . . .

Algebraic eigenvalue problem

\[ T_{\Delta x} y = \lambda_{\Delta x} y \]

Smallest eigenvalue

\[ \lambda_{\Delta x} = -\pi^2 + O(\Delta x^2) \]

The first few eigenvalues are well approximated, but the approximation gradually gets worse.
Discrete Sturm–Liouville. Computation

First three \((N = 19)\) eigenvectors of \(T_{\Delta x}\)
Discrete Sturm–Liouville. Eigenvalues $N = 19$

Discrete eigenvalues $\lambda_{\Delta x}$: 
-9.8493, -39.1548, -87.1948

Exact eigenvalues $\lambda$: 
-9.8696, -39.4784, -88.8264

Relative errors: 
0.21%, 0.82%, 1.63%

- Lowest eigenvalues are more accurate
- Good approximations for $\sqrt{N}$ first eigenvalues

(Here approximately first 4 – 5 modes)
Discrete Sturm–Liouville. High modes

Eigenvectors 7, 13, 19 ($N = 19$) of $T_{\Delta x}$
Discrete Sturm–Liouville. High modes

Eigenvectors 7, 13, 19 \((N = 19)\) of \(T_{\Delta x}\)
5. Toeplitz matrices

A **Toeplitz matrix** is constant along diagonals

**Example** (symmetric)

\[ T_{\Delta x} = \frac{1}{\Delta x^2} \begin{pmatrix} 
-2 & 1 & 0 & \ldots \\
1 & -2 & 1 \\
1 & -2 & 1 \\
\vdots \\
\vdots & 0 & 1 & -2 
\end{pmatrix} \]
Toeplitz matrices . . .

Much is known about Toeplitz matrices

- Eigenvalues
- Norms
- Inverses
- etc.

They can be generated in MATLAB using the built-in function \texttt{toeplitz}
Eigenvalues of Toeplitz matrices

Example  Solve the eigenvalue problem $Ty = \lambda y$ for

$$T = \begin{pmatrix}
-2 & 1 & 0 & \ldots \\
1 & -2 & 1 & \\
1 & -2 & 1 & \\
\vdots & \vdots & \ddots & \\
\ldots & 0 & 1 & -2
\end{pmatrix}$$

Note  $\lambda[T] = -2 + \lambda[S]$
Eigenvalues . . .

. . . the problem gets simplified

\[
S y = \begin{pmatrix}
0 & 1 & 0 & \ldots \\
1 & 0 & 1 \\
1 & 0 & 1 \\
\vdots & & & & 1 \\
\ldots & 0 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
y_1 \\
y_2 \\
\vdots \\
y_N
\end{pmatrix} = \lambda y
\]

Find the eigenvalues of \( S \)!
Eigenvalues . . . and difference equations!

Consider the \( n^{\text{th}} \) equation of \( Sy = \lambda y \):

\[
y_{n+1} + y_{n-1} = \lambda y_n
\]

**Linear difference equation** with boundary values

\[
y_0 = 0; \quad y_{N+1} = 0
\]

**Characteristic equation**

\[
z^2 - \lambda z + 1 = 0
\]
Roots of \( z^2 - \lambda z + 1 = 0 \) are \( z \) and \( 1/z \) (product 1)

General solution \( y_n = \alpha z^n + \beta z^{-n} \)
Eigenvalues . . . characteristic equation

Roots of $z^2 - \lambda z + 1 = 0$ are $z$ and $1/z$ (product 1)

General solution $y_n = \alpha z^n + \beta z^{-n}$

Boundary condition $y_0 = 0 = \alpha + \beta$ \Rightarrow

Solution $y_n = \alpha(z^n - z^{-n})$
Eigenvalues ... characteristic equation

**Roots** of \( z^2 - \lambda z + 1 = 0 \) are \( z \) and \( 1/z \) (product 1)

**General solution** \( y_n = \alpha z^n + \beta z^{-n} \)

**Boundary condition** \( y_0 = 0 = \alpha + \beta \) \( \Rightarrow \)

**Solution** \( y_n = \alpha (z^n - z^{-n}) \)

**Boundary condition**
\[
y_{N+1} = 0 = \alpha(z^{N+1} - z^{-(N+1)}) \quad \Rightarrow \quad z^{2(N+1)} = 1
\]
Eigenvalues ... characteristic equation

Roots of \( z^2 - \lambda z + 1 = 0 \) are \( z \) and \( 1/z \) (product 1)

General solution \( y_n = \alpha z^n + \beta z^{-n} \)

Boundary condition \( y_0 = 0 = \alpha + \beta \) \( \Rightarrow \)

Solution \( y_n = \alpha(z^n - z^{-n}) \)

Boundary condition
\( y_{N+1} = 0 = \alpha(z^{N+1} - z^{-(N+1)}) \) \( \Rightarrow \) \( z^{2(N+1)} = 1 \)

Roots \( z_k = \exp\left(\frac{k\pi i}{N + 1}\right) \quad k = 1 : N \)
Eigenvalues . . .

**Sum of the roots** of \( z^2 - \lambda z + 1 = 0 \) are

\[
\lambda_k = z_k + 1/z_k \quad \Rightarrow
\]

\[
\lambda_k[S] = \exp\left(\frac{k\pi i}{N + 1}\right) + \exp\left(-\frac{k\pi i}{N + 1}\right) = 2 \cos \frac{k\pi}{N + 1}
\]
Eigenvalues . . .

Sum of the roots of $z^2 - \lambda z + 1 = 0$ are

$$\lambda_k = z_k + 1/z_k \implies$$

$$\lambda_k[S] = \exp \left( \frac{k\pi i}{N + 1} \right) + \exp \left( -\frac{k\pi i}{N + 1} \right) = 2 \cos \frac{k\pi}{N + 1}$$

Hence

$$\lambda_k[T] = -2 + 2 \cos \frac{k\pi}{N + 1} = -4 \sin^2 \frac{k\pi}{2(N + 1)}$$
Eigenvalues of Toeplitz matrices

**Theorem** The $N \times N$ Toeplitz matrix

$$T = \begin{pmatrix}
-2 & 1 & 0 & \ldots \\
1 & -2 & 1 & \\
1 & -2 & 1 & \\
\ldots & & & \\
\ldots & 0 & 1 & -2
\end{pmatrix}$$

has $N$ real eigenvalues ($k = 1 : N$)

$$\lambda_k[T] = -4 \sin^2 \frac{k\pi}{2(N+1)} \in (-4, 0)$$
Consider the operator approximation

\[
\frac{d^2}{dx^2} \leftrightarrow \frac{1}{\Delta x^2} T
\]

on \( x \in [0, 1] \), with \( \Delta x = 1/(N + 1) \)

**Corollary** \( \text{The eigenvalues of } T_{\Delta x} := T/\Delta x^2 \text{ are} \)

\[
\lambda_k[T_{\Delta x}] = -4(N + 1)^2 \sin^2 \frac{k\pi}{2(N + 1)} \approx -k^2 \pi^2
\]

for \( k \ll N \)
What are the eigenvalues of $d^2/dx^2$ on $[0, 1]$?

Consider the Sturm–Liouville problem

$$u'' = \lambda u \; ; \; u(0) = u(1) = 0$$

Solutions

$$u(x) = A \sin \sqrt{-\lambda} x + B \cos \sqrt{-\lambda} x$$

Boundary conditions

$$B = 0 \; \text{and} \; A \sin \sqrt{-\lambda} = 0$$
What are the eigenvalues of $d^2/dx^2$ on $[0, 1]$?

Consider the Sturm–Liouville problem

$$u'' = \lambda u ; \quad u(0) = u(1) = 0$$

Solutions $u(x) = A \sin \sqrt{-\lambda} x + B \cos \sqrt{-\lambda} x$

Boundary conditions $B = 0$ and $A \sin \sqrt{-\lambda} = 0$

**Theorem**  *The eigenvalues are* $\lambda_k[d^2/dx^2] = -k^2 \pi^2$

**Note** $k \in \mathbb{Z}^+$
What are the norms of $T$?

Lemma  For a symmetric matrix $A$, it holds
\[ \|A\|_2 = \max_k |\lambda_k| \]
What are the norms of $T$?

Lemma  For a symmetric matrix $A$, it holds

$$\|A\|_2 = \max_k |\lambda_k|$$

Lemma  For a symmetric matrix $A$, it holds

$$\mu_2[A] = \max_k \lambda_k$$

(Both results actually hold for normal matrices)
Proofs: Norm

Definition

\[ \| A \|_2^2 = \max_{x^T x \neq 0} \frac{x^T A^T A x}{x^T x} \]

Find stationary points of the Rayleigh quotient of \( A^T A \), given by

\[ \rho(x) = \frac{x^T A^T A x}{x^T x} \]

\[ \text{grad}_x \rho(x) = \frac{2 A^T A x x^T x - 2 x x^T A^T A x}{(x^T x)^2} : = 0 \]

\[ A^T A x = \rho(x) x \quad \Rightarrow \quad A^2 x = \rho(x) x \]
Proofs: Norm . . .

So $\rho(x) = \lambda^2$, where $\lambda$ is an eigenvalue of $A$

Therefore $\|A\|_2^2 = \max |\lambda[A]|^2$ or

$$\|A\|_2 = \max |\lambda[A]|$$

when $A$ is *symmetric*
Proofs: Logarithmic norm

Definition

\[ \mu_2[A] = \max_{x^T x \neq 0} \frac{x^T Ax}{x^T x} \]

Find stationary points of the Rayleigh quotient of \( A \), given by

\[ \rho(x) = \frac{x^T Ax}{x^T x} \]

\[ \nabla_x \rho(x) = \frac{[(A + A^T)xx^T x - 2xx^T Ax]}{(x^T x)^2} : = 0 \]

\[ \frac{1}{2}(A + A^T)x = \rho(x)x \quad \Rightarrow \quad Ax = \rho(x)x \]
Proofs: Logarithmic norm . . .

So \( \rho(x) = \lambda \), where \( \lambda \) is an eigenvalue of \( A \).

Therefore \( \mu_2[A] = \max \lambda[A] \) when \( A \) is \textit{symmetric}.

For symmetric matrices we have proved

\[
\|A\|_2 = \max_k |\lambda_k| \quad \mu_2[A] = \max_k \lambda_k
\]
What are the norms of $T_{\Delta x}$?

Eigenvalues of $T_{\Delta x} = T / \Delta x^2$ are

$$\lambda_k[T_{\Delta x}] = -4(N + 1)^2 \sin^2 \frac{k\pi}{2(N + 1)}$$

So $\|T_{\Delta x}\|_2 = |\lambda_N|$ and $\mu_2[T_{\Delta x}] = \lambda_1$

**Theorem**  The Euclidean norms of $T_{\Delta x}$ are

$$\|T_{\Delta x}\|_2 \approx \frac{4}{\Delta x^2} \quad \mu_2[T_{\Delta x}] \approx -\pi^2$$
The norm of $T_{\Delta x}^{-1}$

Recall that $\mu[A] < 0 \implies \|A^{-1}\| \leq -1/\mu[A]$

Approximate $y'' = f(x)$ with $y(0) = y(1) = 0$ by

$$T_{\Delta x}u = q$$

Note that $\mu_2[T_{\Delta x}] \approx -\pi^2$ then implies that this problem has a unique solution, as

$$\|T_{\Delta x}^{-1}\|_2 \approx \frac{1}{\pi^2}$$
What norms to use. RMS and Euclidean norms

The norm of a function is measured in the $L^2$ norm

$$\|l\|_2^2 = \int_0^1 l(x)^2 \, dx$$

A corresponding discrete function (vector) is then measured in the root mean square (RMS) norm

$$\|l(x)\|_{\Delta x}^2 = \sum_{i=1}^{N} l(x_i)^2 \Delta x = \frac{1}{N+1} \sum_{i=1}^{N} l(x_i)^2 = \frac{1}{N+1} \|l(x)\|_2^2$$

Important! Note that $\|T_{\Delta x}^{-1}\|_{\Delta x} \equiv \|T_{\Delta x}^{-1}\|_2$
Solution and error bounds

Approximate $y'' = f(x)$ with $y(0) = y(1) = 0$ by

$$T_{\Delta x}u = q$$

Convergence analysis will show

**Theorem** $\mu_2[T_{\Delta x}] \approx -\pi^2$ implies a *unique solution* with

$$\|u\|_{\Delta x} \lesssim \frac{\|q\|_{\Delta x}}{\pi^2} \quad \|e(x)\|_{\Delta x} \lesssim \frac{\|l(x)\|_{\Delta x}}{\pi^2}$$

Solution–data \quad Global–local error
6. Convergence of finite difference methods

Basic problem

\[ y'' = f(x, y) \]
\[ y(0) = \alpha; \quad y(1) = \beta \]

Equidistant discretization

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = f(x_i, y_i) \]
\[ y_0 = \alpha; \quad y_{N+1} = \beta \]
Error definitions

Local error

Insert exact solution $y(x)$ into discretization:

$$\frac{y(x_{i-1}) - 2y(x_i) + y(x_{i+1})}{\Delta x^2} = f(x_i, y(x_i)) - l(x_i)$$

Taylor expansion, using $f(x_i, y(x_i)) = y''(x_i)$:

$$-l(x_i) = 2 \left( \frac{\Delta x^2}{4!} y^{(4)}(x_i) + \frac{\Delta x^4}{6!} y^{(6)}(x_i) + \ldots \right)$$

Only even powers of $\Delta x$ due to symmetry
Global error

**Definition**  The global error is defined  
\[ e(x_i) = y_i - y(x_i) \]

**Convergence**  Will show that  \( e(x) \to 0 \) as  \( \Delta x \to 0 \), or more specifically

\[ e(x_i) = c_1 \Delta x^2 + c_2 \Delta x^4 + \ldots \]

Again only *even powers* due to symmetry
Convergence

Assume $f$ is a linear function, ⇒ $F$ is linear ⇒

$$F(y) = 0 \iff T_{\Delta x} y = q$$

with $T_{\Delta x}$ tridiagonal. Then

- **Numerical solution** $T_{\Delta x} y = q$
- **Exact solution** $T_{\Delta x} y(x) = q - l(x)$
Convergence . . .

Solve \( T_{\Delta x} y = q \) formally to get

**Numerically**  \[ y = T_{\Delta x}^{-1} \cdot q \]

**Exact**  \[ y(x) = T_{\Delta x}^{-1} \cdot (q - l(x)) \]

**Global error**  \[ e(x) = T_{\Delta x}^{-1} \cdot l(x) \]

**Error bound**  \[ \| e(x) \|_{\Delta x} \leq \| T_{\Delta x}^{-1} \|_2 \cdot \| l(x) \|_{\Delta x} \]
Matching norms: RMS and Euclidean norms

Note how root mean square (RMS) norm of vector

\[ \| l(x) \|_{\Delta x}^2 = \sum_{1}^{N} l(x_i)^2 \Delta x = \frac{1}{N+1} \sum_{1}^{N} l(x_i)^2 = \frac{1}{N+1} \| l(x) \|_2^2 \]

is matched to the Euclidean matrix norm, by way of

\[ \| T_{\Delta x}^{-1} \|_{\Delta x} \equiv \| T_{\Delta x}^{-1} \|_2 \]

(Prove this relation!)
Recall $\mu_2[T_{\Delta x}] \approx -\pi^2 \Rightarrow \left\| T_{\Delta x}^{-1} \right\|_2 \lesssim 1/\pi^2 \ (\Delta x \to 0)$

Since $\left\| e(x) \right\|_{\Delta x} \leq \left\| T_{\Delta x}^{-1} \right\|_2 \cdot \left\| l(x) \right\|_{\Delta x}$ and 
$\left\| l \right\|_{\Delta x} = \gamma_1 \Delta x^2 + \gamma_2 \Delta x^4 \ldots \text{ we have}$

$$\left\| e \right\|_{\Delta x} \leq C \cdot \left\| l \right\|_{\Delta x} = c_1 \Delta x^2 + c_2 \Delta x^4 + \ldots$$

... and we have convergence as $\Delta x \to 0!$ :)
Convergence: Lax’ principle

Conclusion

**Consistency:** local error \( l \to 0 \) as \( \Delta x \to 0 \)

**Stability:** \( \| T_{\Delta x}^{-1} \|_2 \leq C \) as \( \Delta x \to 0 \)

**Convergence:** global error \( e \to 0 \) as \( \Delta x \to 0 \)

**Theorem** (Lax’ Principle)

**Consistency + Stability \( \Rightarrow \) Convergence**

(“Fundamental theorem of numerical analysis”)
7. Differential operators. Integration by parts

Logarithmic norm of matrix:

\[ \mu_2[A] = \max_{x \neq 0} \frac{x^T Ax}{x^T x} \quad \Rightarrow \quad x^T Ax \leq \mu_2[A] \cdot x^T x \]

For \( d^2/dx^2 \), introduce the inner product

\[ \langle u, v \rangle = \int_0^1 \bar{u}(x)v(x) \, dx \quad \Rightarrow \quad \| u \|_2^2 = \langle u, u \rangle \]
The logarithmic norm of $d^2/dx^2$

Can we find a constant $\mu_2[d^2/dx^2]$ such that

$$\langle u, u'' \rangle \leq \mu_2[d^2/dx^2] \cdot \| u \|_2^2$$

for all functions $u \in C^2_0[0, 1]$?

Yes and $\mu_2[d^2/dx^2] = -\pi^2$
Integration by parts

\[ \int_0^1 uv' \, dx = [uv]^1_0 - \int_0^1 u'v \, dx \]

Because \( u(0) = u(1) = 0 \), this can be written

\[ \langle u, v' \rangle = -\langle u', v \rangle \]

Apply to \( d^2/dx^2 \) \( \Rightarrow \)

\[ \langle u, u'' \rangle = -\langle u', u' \rangle = -\|u'\|_2^2 \]
Sobolev’s lemma

**Lemma** For all functions $u$ with $u(0) = u(1) = 0$ it holds that

$$\|u'\|_2 \geq \pi \|u\|_2$$

**Proof** Fourier analysis (Parseval’s theorem)

$$u = \sqrt{2} \sum_{k=1}^{\infty} c_k \sin k\pi x \quad \Rightarrow \quad u' = \pi \sqrt{2} \sum_{k=1}^{\infty} k c_k \cos k\pi x$$

implies $\|u'\|_2 \geq \pi \|u\|_2$
Logarithmic norm of $d^2/{dx}^2$ on $[0, 1]$ 

$$\langle u, u'' \rangle = -\langle u', u' \rangle = -\|u'\|_2^2 \leq -\pi^2\|u\|_2^2$$

**Theorem**  The logarithmic norm of $d^2/{dx}^2$ on $C_0^2[0, 1]$ is 

$$\mu_2[d^2/{dx}^2] = -\pi^2$$

**Corollary**  The 2pBVP $u'' = f(x); \; u(0) = u(1) = 0$; has a unique solution with $\|u\|_2 \leq \|f\|_2/\pi^2$
Self-adjoint operators

Definition

\[ \langle v, Au \rangle = \langle A^* v, u \rangle \]

defines the adjoint operator \( A^* \)

Example  For vectors and matrices

\[ \langle v, Au \rangle = v^T A u = (A^T v)^T u = \langle A^* v, u \rangle \]

\( A^T \) is the adjoint of \( A \)

A matrix is self-adjoint ("symmetric") if \( A = A^T \)
Self-adjoint differential operators . . .

**Example** \( \frac{d^2}{dx^2} \) on \( C^2_0[0, 1] \)

Integrate by parts

\[
\langle v, u'' \rangle = -\langle v', u' \rangle = \langle v'', u \rangle
\]

So \( \frac{d^2}{dx^2} \) *is a self-adjoint operator*

More generally,

\[
\frac{d}{dx} \left( p(x) \frac{d}{dx} \right) + q(x)
\]

is self-adjoint on \( C^2_0[0, 1] \)
Eigenvalues of self-adjoint operators . . .

... are real: let $Au = \lambda u$

\[
\lambda \|u\|^2_2 = \langle u, \lambda u \rangle = \langle u, Au \rangle = \langle A^* u, u \rangle \\
= \langle Au, u \rangle = \langle \lambda u, u \rangle = \bar{\lambda} \|u\|^2_2
\]

So $\lambda = \bar{\lambda}$ implies \textit{real eigenvalues}.
Eigenvectors of self-adjoint operators . . .

. . . are orthogonal; let $Au = \lambda u$ and $Av = \mu v$

\[
\lambda \langle v, u \rangle = \langle v, Au \rangle = \langle A^* v, u \rangle = \langle Av, u \rangle = \mu \langle v, u \rangle
\]

So $\lambda - \mu \rangle v, u \rangle = 0 \implies \langle v, u \rangle = 0$ implying that

eigenvectors are orthogonal
Elliptic operators

**Definition**  
An operator is *elliptic* if for all $u \neq 0$  

$$\langle u, Au \rangle > 0$$

**Example**  
$-\frac{d^2}{dx^2}$  
on $C_0^2[0, 1]$

Integrate by parts  

$$-\langle u, u'' \rangle = \langle u', u' \rangle \geq \pi^2 \langle u, u \rangle$$

by Sobolev’s lemma
Elliptic operators . . .

More generally,

$$-rac{d}{dx} \left( p(x) \frac{d}{dx} \right) + q(x)$$

_is elliptic if_ \( p(x) > 0 \) _and_ \( q(x) \geq 0 \)

**Example** Laplace’s equation

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

_\( -\Delta \) is an elliptic operator_
Positive definite operators

**Definition**  An operator is *positive definite* if it is self-adjoint and elliptic

$$\mu_2[-A] < 0$$

**Example**  $-d^2/dx^2$ as $\mu_2[d^2/dx^2] = -\pi^2$ on $C^2_0[0, 1]$

Negative Laplacian $-\Delta$  (leads to FEM theory)
8. From Finite Difference to Finite Element

Start with linear differential equation

\[ Au = f \quad + \quad \text{boundary conditions} \]

Finite Difference Method (FDM). The main idea

*Replace functions \( u \) and \( f \) by vectors* and *differential operator \( A \) by matrix* to get a linear system of equations

**Example**

\[ \frac{d^2}{dx^2} u = f(x) \quad \Rightarrow \quad T_{\Delta x} u = f \]
Finite Elements and the Galerkin method

Galerkin Method. The main idea

Approximate function \( u \) by polynomial and keep differential operator \( A \) as is!

Take some polynomial \( v \) satisfying boundary conditions. Insert into original equation to get \( Av \approx f \)

**Question** Which polynomial gives the best approximation?

**Answer** Choose \( v \) to minimize the residual \( \| Av - f \|_2 \)
Best approximation = least squares

Let \( \{ \varphi_j \} \) be a polynomial basis, and make the ansatz

\[
v(x) = \sum_{j=1}^{N} c_j \varphi_j(x)
\]

Minimizing \( \| Av - f \|_2 \) is equivalent to requiring that

the residual is orthogonal to each and every \( \varphi_i \)

\[
\langle \varphi_i, Av - f \rangle = 0 \quad \forall i
\]

This is the least-squares approximation!
Best approximation . . .

As $\mathcal{A}$ is linear,

$$\mathcal{A}v = \mathcal{A} \sum_{j=1}^{N} c_j \varphi_j = \sum_{j=1}^{N} c_j \mathcal{A} \varphi_j$$

Then

$$\langle \varphi_i, \mathcal{A}v - f \rangle = 0 \iff \sum_{j=1}^{N} \langle \varphi_i, \mathcal{A} \varphi_j \rangle c_j = \langle \varphi_i, f \rangle$$

This is a linear system of equations $\sum a_{ij} c_j = b_i$ or $Ac = b$, with matrix and vector elements

$$a_{ij} = \langle \varphi_i, \mathcal{A} \varphi_j \rangle \quad \quad b_i = \langle \varphi_i, f \rangle$$
Weak formulation. The problem \(-u'' = f\)

If \(-u'' = f\) then for all \(v\)

\[\langle v, -u'' \rangle = \langle v, f \rangle\]

Integrate by parts and use Dirichlet boundary data to get

**Weak formulation** \[\langle v', u' \rangle = \langle v, f \rangle\quad \forall v\]

The weak formulation requires \(u\) to be once continuously differentiable, not twice.
Weak formulation and energy norm

Definition  The energy norm is defined by

\[ a(v, u) = \langle v', u' \rangle \]

and the weak formulation can be written: Find a function \( u \) such that for all test functions \( v \) it holds

\[ a(v, u) = \langle v, f \rangle \]

What functions? Choose a polynomial space \( \mathcal{V} \) with basis \( \{ \varphi_j \} \), satisfying the boundary conditions, and require \( v \in \mathcal{V} \) and \( u \in \mathcal{V} \), all defined on suitable grid \( \{ x_i \} \)
Example. The Finite Element Method (FEM)

Given grid \( \{x_i\} \), choose \textit{piecewise linear basis polynomials} \n
\[ \varphi_j(x_i) = 1 \text{ if } i = j, \text{ otherwise } 0 \]

\[ v(x) = \sum_{j=1}^{N} c_j \varphi_j(x) \]

\text{Note that } v(x_i) = c_i \approx u(x_i)
Galerkin Finite Element Method for $-u'' = f$

Best approximation $a(v, u) = \langle v, f \rangle$, with $u, v \in \mathcal{V}$, leads to

$$a(\varphi_i, \sum_{j=1}^{N} c_j \varphi_j) = \langle \varphi_i, f \rangle$$

which is equivalent to the \textit{finite element equation} $Kc = b$

$$\sum_{j=1}^{N} \langle \varphi'_i, \varphi'_j \rangle c_j = \langle \varphi_i, f \rangle \quad \forall \varphi_i \in \mathcal{V}$$

The \textit{stiffness matrix} $K$ with elements $\{\langle \varphi'_i, \varphi'_j \rangle\}_{i,j=1}^{N}$ can be computed as soon as the basis $\{\varphi_j\}$ has been constructed.

The right-hand side vector $b$ depends on the data $f$. 

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Numerical Methods for Differential Equations – p. 81/86
Assume an equidistant grid with spacing $\Delta x$. Note that 

$$\varphi'_i(x) = 1/\Delta x \quad \text{on} \quad [x_{i-1}, x_i]$$

$$\varphi'_i(x) = -1/\Delta x \quad \text{on} \quad [x_i, x_{i+1}]$$

$$\varphi'_i(x) = 0 \quad \text{elsewhere}$$

Then

$$\langle \varphi'_i, \varphi'_i \rangle = \int_{x_{i-1}}^{x_{i+1}} \frac{1}{\Delta x^2} \, dx = \frac{2}{\Delta x}$$

$$\langle \varphi'_i, \varphi'_{i+1} \rangle = \int_{x_{i}}^{x_{i+1}} \frac{-1}{\Delta x^2} \, dx = \frac{-1}{\Delta x}$$
Stiffness matrix

For equidistant grid with spacing $\Delta x$ the \textit{stiffness matrix} is

$$K_{\Delta x} = \frac{1}{\Delta x} \text{tridiag}(-1 \quad 2 \quad -1)$$

\textbf{Note}

1) The stiffness matrix is $K_{\Delta x} = -\Delta x \cdot T_{\Delta x}$

2) It is \textit{positive definite}, therefore nonsingular

3) Smallest eigenvalue $\lambda_1[K_{\Delta x}] \approx \pi^2 \Delta x$
Mass matrix

Compute RHS integrals using numerical integration

\[ \langle \varphi_i, f \rangle \approx \langle \varphi_i, \sum_{j=0}^{N} f_j \varphi_j \rangle = \sum_{k=-1}^{1} f_{i+k} \langle \varphi_i, \varphi_{i+k} \rangle \]

Need to compute \( \langle \varphi_i, \varphi_{i+k} \rangle = \int_{x_{i-1}}^{x_{i+1}} \varphi_i(x) \varphi_{i+k}(x) \, dx \)

The integrals are \( \langle \varphi_i, \varphi_i \rangle = 2\Delta x / 3 \) and \( \langle \varphi_i, \varphi_{i+1} \rangle = \Delta x / 6 \)

For equidistant grid with spacing \( \Delta x \) the \textit{mass matrix} is

\[ B_{\Delta x} = \frac{\Delta x}{6} \text{tridiag}(1 \quad 4 \quad 1) \]
Assembling the system of equations

Final finite element equations is a tridiagonal linear system

\[ K_{\Delta x} c = B_{\Delta x} f \]

with *stiffness matrix*

\[ K_{\Delta x} = \frac{1}{\Delta x} \text{tridiag}(1 - 2 1) \]

and *mass matrix*

\[ B_{\Delta x} = \frac{\Delta x}{6} \text{tridiag}(1 4 1) \]
Advantages of the Finite Element Method

- Produces “continuous solution” not only on grid points
- Can also use basis of higher degree splines
- Can easily use nonuniform grids
- Boundary conditions built into test functions
- In PDEs, easy to work with complex geometries
- Rich theoretical foundation