Numerical Methods for Differential Equations

Chapter 4: Two-point boundary value problems

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Textbooks: *A First Course in the Numerical Analysis of Differential Equations*, by Arieh Iserles and *Introduction to Mathematical Modelling with Differential Equations*, by Lennart Edsberg

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 ($y' = \mathrm{d}y/\mathrm{d}x$)

First order approximations

Forward difference

$$y'(x) = \frac{y(x + \Delta x) - y(x)}{\Delta x} + \mathrm{O}(\Delta x)$$

Backward difference

$$y'(x) = \frac{y(x) - y(x - \Delta x)}{\Delta x} + \mathrm{O}(\Delta x)$$

Approximation of derivatives . . .

Second order approximations

Symmetric difference quotients

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

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

Derivatives → finite differences → matrices

Matrix representation of *forward difference*

$$y'(x) = \frac{y(x+\Delta x) - y(x)}{\Delta x} + \mathrm{O}(\Delta x)$$

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

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

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 $y = (1 \quad 1 \quad 1 \ldots 1)^{\mathrm{T}}$

Compare nullspace of $\mathrm{d}/\mathrm{d}x$*:* $y = 1 \ \Rightarrow\ y' \equiv 0$

Analogous result for backward difference

Derivatives . . . matrices

Central difference

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

Matrix representation

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

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:

$\bar{y} = (1 \quad 1 \quad 1 \ldots 1)^{\mathrm{T}}$ and $\tilde{y} = (1 \ -1 \quad 1 \ -1 \ldots 1)^{\mathrm{T}}$

Derivatives . . . matrices

“False” nullspace $\tilde{y} = (1\ -1\quad 1\ -1 \ldots 1)^{\mathrm{T}}$ *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 $\bar{y} = (1 \quad 1 \ldots 1)^{\mathrm{T}}$
and $\hat{y} = (0 \quad 1 \quad 2 \quad 3 \ldots N+1)^{\mathrm{T}}$

2nd order derivatives ...

Nullspace of $\mathrm{d}^2/\mathrm{d}x^2$:

$y = 1$ and $y = x$ both have $y'' \equiv 0$

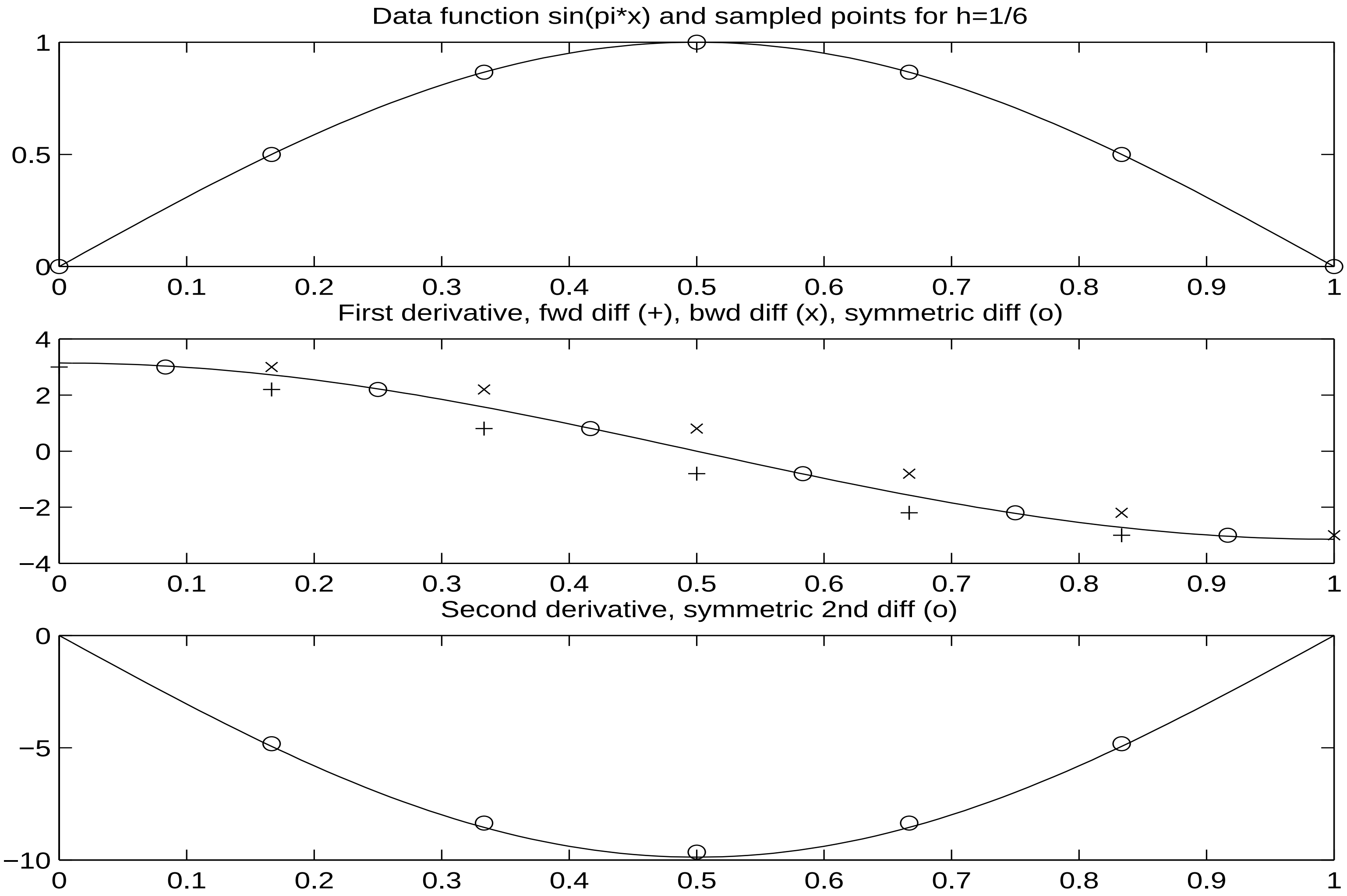
Compare difference equation $y_{n+1} - 2y_n + y_{n-1} = 0$, with characteristic equation

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

and solutions $\bar{y}_n = 1$ and $\hat{y}_n = n$, respectively

Numerical differentiation

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



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

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

$$y_0 = \alpha; \qquad y_{N+1} = \beta$$

Discrete 2pBVP

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

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

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

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

$$F'(y) = \text{tridiag}\,(1/\Delta x^2\,, \quad -2/\Delta x^2 + \frac{\partial f}{\partial y_i}\,, \qquad 1/\Delta x^2)$$

is *tridiagonal*, and

- Super- and subdiagonal elements $1/\Delta x^2$
- Diagonal elements $-2/\Delta x^2 - \partial f/\partial y_i$
- 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. $\|F'(y^{(k)})^{-1}\| \le C'$
2. $\|F''(y^{(k)})\| \le C''$
3. $\|y^{(0)} - y\| < \varepsilon$ (close enough starting value)

Then convergence is quadratic

$$\|y^{(k+1)} - y\| \le C \cdot \|y^{(k)} - y\|^2$$

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!*

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

$$\Rightarrow \quad y_{N+1} := \frac{(2c - \Delta x)y_N + 2\kappa\Delta x}{2c + \Delta x}$$

4. Sturm–Liouville eigenvalue problems

Diffusion problem

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

Separation of variables (one space dimension)

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

Sturm–Liouville eigenvalue problem

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\,\frac{\mathrm{d}y}{\mathrm{d}x}\right) - \lambda y = 0\,; \qquad y(a) = 0\,,\ \ y(b) = 0$$

Sturm–Liouville eigenvalue problem...

Wave equation

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

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

$$-\omega^2 y = c^2 y''$$

Sturm–Liouville eigenvalue problem

$$y'' = \lambda y \quad \text{with} \quad \lambda = -\omega^2/c^2$$

Sturm–Liouville eigenvalue problem…

Find *eigenvalues* λ and *eigenfunctions* $y(x)$ with

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

Discretization *Matrix eigenvalue problem*

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

Note Analytic eigenvalue problem converts to algebraic!

Sturm–Liouville problem. Discretization

$$\frac{p_{i-1/2}y_{i-1} - (p_{i-1/2} + p_{i+1/2})y_i + p_{i+1/2}y_{i+1}}{\Delta x^2} = \lambda_{\Delta x} y_i$$

$$y_0 = y_{N+1} = 0$$

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

$$A \sin\sqrt{-\lambda} = 0$$
$$A \neq 0 \quad \Rightarrow \quad \sqrt{-\lambda_n} = n\pi \qquad n = 1,\ 2, \ldots$$

Simple Sturm–Liouville example . . .

$$y'' = \lambda y$$
$$y(0) = y(1) = 0$$

Eigenvalues $\lambda_n = -n^2\pi^2$, $n = 1, 2, \ldots$

Eigenfunctions $y_n(x) = \sin n\pi x$

Discrete Sturm–Liouville. Same example

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

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

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

Tridiagonal $N \times N$ matrix formulation

$$\frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \lambda_{\Delta x} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$

Discrete Sturm–Liouville . . .

Algebraic eigenvalue problem

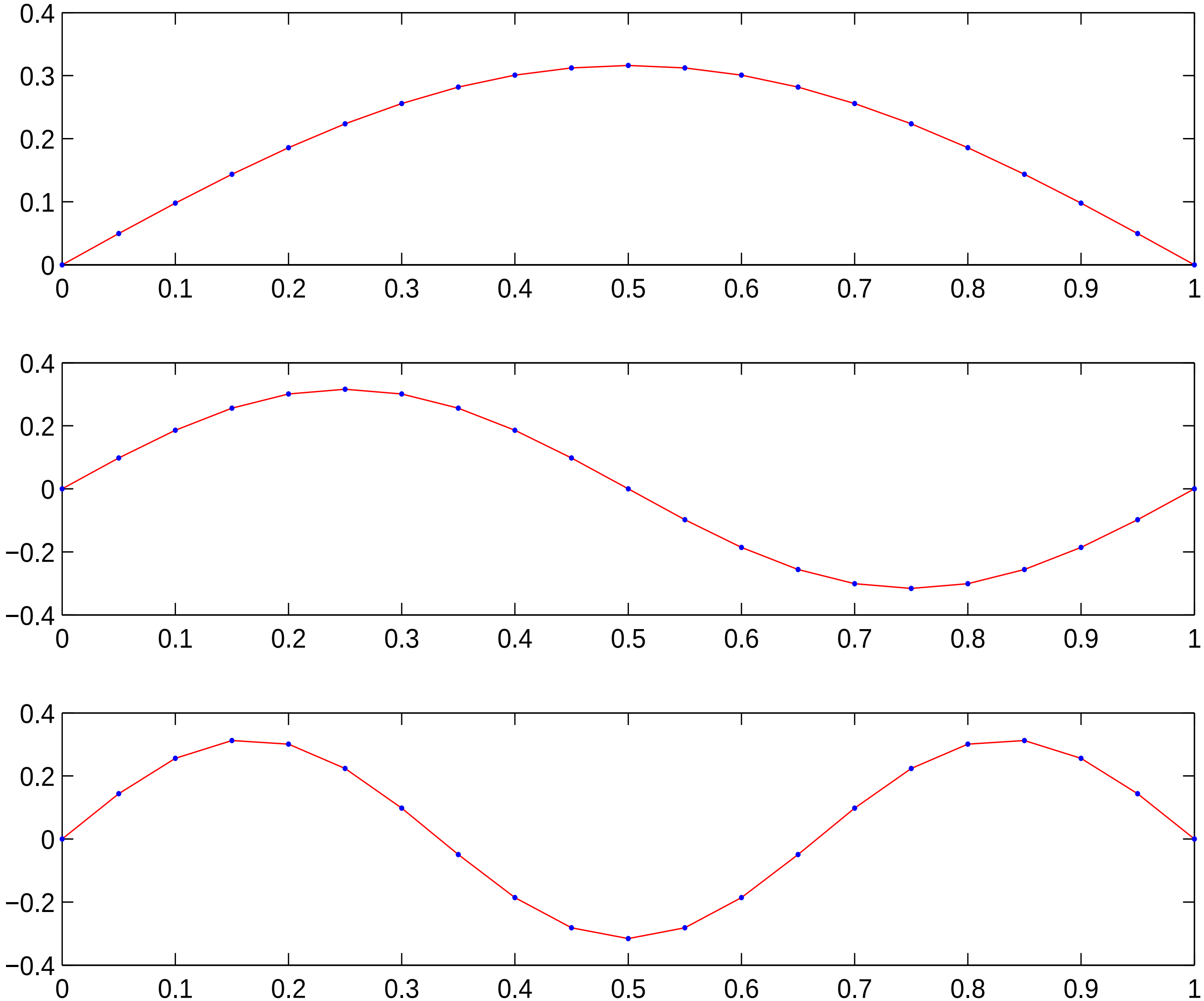
$$T_{\Delta x}\, y = \lambda_{\Delta x}\, y$$

Smallest eigenvalue $\lambda_{\Delta x} = -\pi^2 + \mathrm{O}(\Delta x^2)$

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 $N = 19$

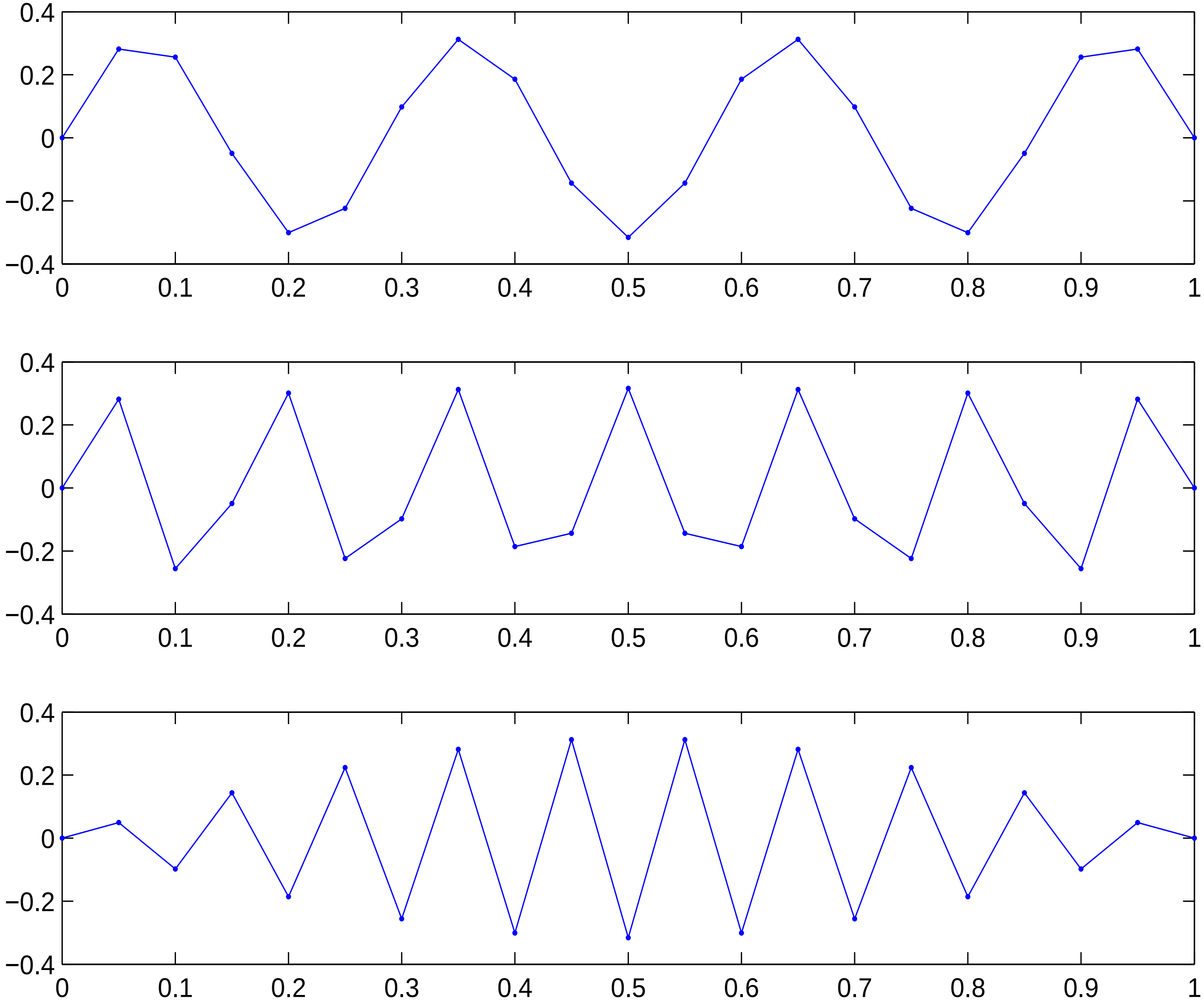
Discrete eigenvalues $\lambda_{\Delta x}$	-9.8493	-39.1548	-87.1948
Exact eigenvalues λ	-9.8696	-39.4784	-88.8264
Relative errors	0.21%	0.82%	1.63%

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

  (Here approximately first 4 – 5 modes)

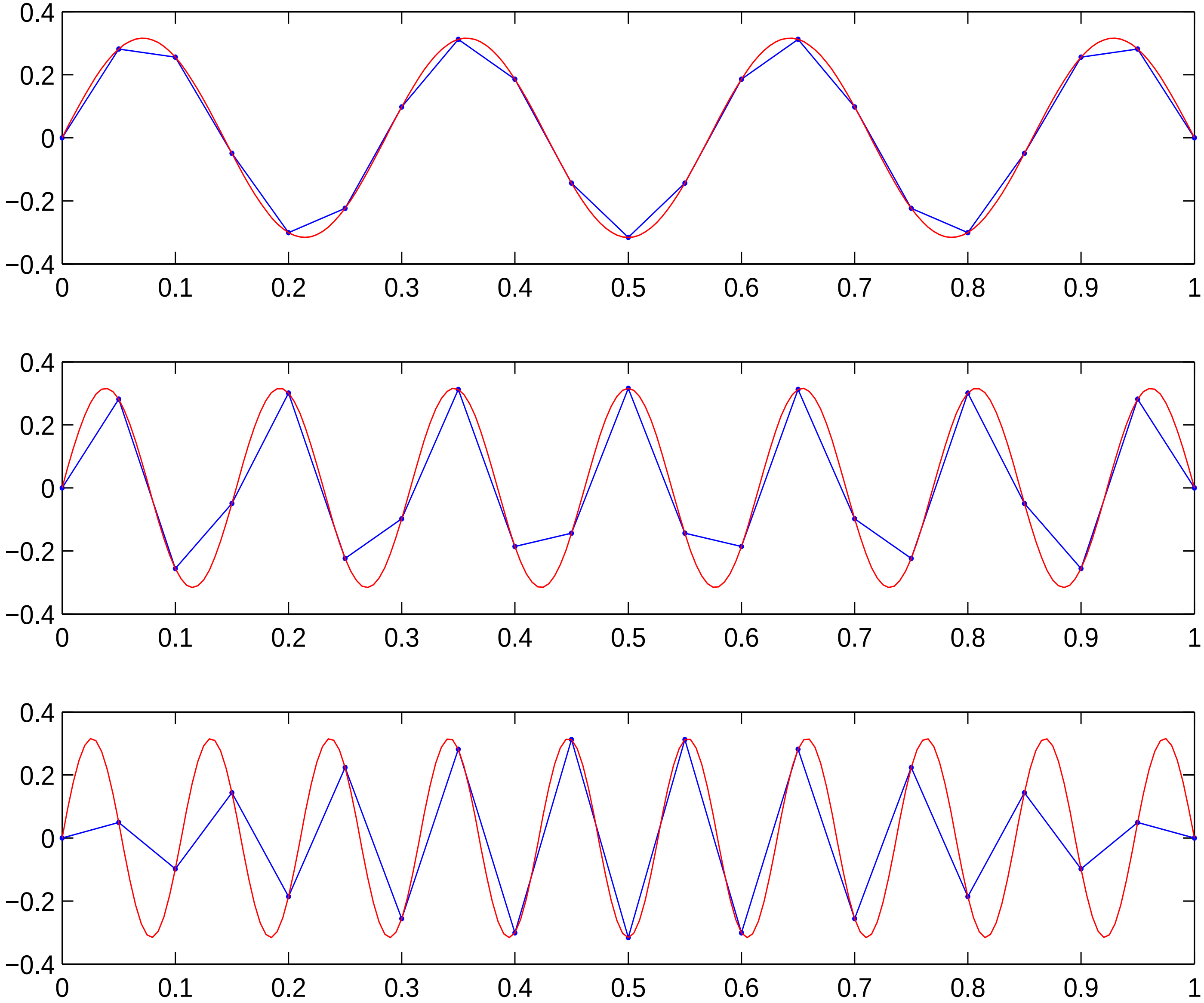
Discrete Sturm–Liouville. High modes

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)

$$T_{\Delta x} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & \dots & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & & \ddots & & \\ & \dots & 0 & 1 & -2 \end{pmatrix}$$

Toeplitz matrices . . .

Much is known about Toeplitz matrices

- *Eigenvalues*
- *Norms*
- *Inverses*
- *etc.*

They can be generated in MATLAB using the built-in function **`toeplitz`**

Eigenvalues of Toeplitz matrices

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

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

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

Eigenvalues . . .

. . . the problem gets simplified

$$Sy = \begin{pmatrix} 0 & 1 & 0 & \dots & \\ 1 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & & \ddots & 1 \\ & \dots & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \\ y_N \end{pmatrix} = \lambda y$$

Find the eigenvalues of S!

Eigenvalues . . . and difference equations!

Consider the n^{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

$$z^2 - \lambda z + 1 = 0$$

Eigenvalues . . . characteristic equation

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

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

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 $y_0 = 0 = \alpha + \beta \quad \Rightarrow$

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 $y_0 = 0 = \alpha + \beta \quad \Rightarrow$

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

Boundary condition

$$y_{N+1} = 0 = \alpha\big(z^{N+1} - z^{-(N+1)}\big) \quad \Rightarrow \quad z^{2(N+1)} = 1$$

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 $y_0 = 0 = \alpha + \beta \quad \Rightarrow$

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

Boundary condition

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

Roots $$z_k = \exp\left(\frac{k\pi \mathrm{i}}{N+1}\right) \qquad k = 1 : N$$

Eigenvalues . . .

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

$$\lambda_k = z_k + 1/z_k \quad \Rightarrow$$

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

Eigenvalues . . .

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

$$\lambda_k = z_k + 1/z_k \quad \Rightarrow$$

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

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*

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

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

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

Eigenvalues of Toeplitz matrices . . .

Consider the operator approximation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} \quad \leftrightarrow \quad \frac{1}{\Delta x^2}T$$

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

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

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

for $k \ll N$

What are the eigenvalues of $\mathrm{d}^2/\mathrm{d}x^2$ 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 $A \sin \sqrt{-\lambda} = 0$

What are the eigenvalues of $\mathrm{d}^2/\mathrm{d}x^2$ 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* $\lambda_k[\mathrm{d}^2/\mathrm{d}x^2] = -k^2\pi^2$

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

$$\|A\|_2^2 = \max_{x^{\mathrm{T}}x \neq 0} \frac{x^{\mathrm{T}}A^{\mathrm{T}}Ax}{x^{\mathrm{T}}x}$$

Find stationary points of the *Rayleigh quotient* of $A^{\mathrm{T}}A$, given by $\rho(x) = x^{\mathrm{T}}A^{\mathrm{T}}Ax/x^{\mathrm{T}}x$

$$\mathrm{grad}_x \rho(x) = (2A^{\mathrm{T}}Axx^{\mathrm{T}}x - 2xx^{\mathrm{T}}A^{\mathrm{T}}Ax)/(x^{\mathrm{T}}x)^2 := 0$$

$$A^{\mathrm{T}}Ax = \rho(x)x \quad \Rightarrow \quad A^2x = \rho(x)x$$

Proofs: Norm . . .

So $\rho(x) = \lambda^2$, where λ 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

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

Find stationary points of the *Rayleigh quotient* of A, given by $\rho(x) = x^{\mathrm{T}}Ax/x^{\mathrm{T}}x$

$$\mathrm{grad}_x \rho(x) = [(A + A^{\mathrm{T}})xx^{\mathrm{T}}x - 2xx^{\mathrm{T}}Ax]/(x^{\mathrm{T}}x)^2 := 0$$

$$\frac{1}{2}(A + A^{\mathrm{T}})x = \rho(x)x \quad \Rightarrow \quad Ax = \rho(x)x$$

Proofs: Logarithmic norm . . .

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

Therefore $\mu_2[A] = \max \lambda[A]$ when A is *symmetric*.

For symmetric matrices we have proved

$$\|A\|_2 = \max_k |\lambda_k| \qquad \mu_2[A] = \max_k \lambda_k$$

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*

$$\|T_{\Delta x}\|_2 \approx \frac{4}{\Delta x^2} \qquad \mu_2[T_{\Delta x}] \approx -\pi^2$$

The norm of $T_{\Delta x}^{-1}$

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

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

$$\|T_{\Delta x}^{-1}\|_2 \lessapprox \frac{1}{\pi^2}$$

What norms to use. RMS and Euclidean norms

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

$$\|l\|_2^2 = \int_0^1 l(x)^2 \mathrm{d}x$$

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

$$\|l(x)\|_{\Delta x}^2 = \sum_1^N l(x_i)^2 \Delta x = \frac{1}{N+1} \sum_1^N l(x_i)^2 = \frac{1}{N+1} \|l(x)\|_2^2$$

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

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

Solution–data 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 $f(x_i, y(x_i)) = y''(x_i)$:

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

Only *even powers* of Δx 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 specificallly

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

Again only *even powers* due to *symmetry*

Convergence

Assume f is a linear function, $\Rightarrow$ F is linear $\Rightarrow$

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

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

Numerical solution $\quad T_{\Delta x} y = q$

Exact solution $\quad T_{\Delta x} y(x) = q - l(x)$

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!)

Convergence . . .

Recall $\mu_2[T_{\Delta x}] \approx -\pi^2 \;\Rightarrow\; \|T_{\Delta x}^{-1}\|_2 \lessapprox 1/\pi^2$ $(\Delta x \to 0)$

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

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

. . . 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:

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

For $\mathrm{d}^2/\mathrm{d}x^2$, introduce the *inner product*

$$\langle u, v \rangle = \int_0^1 \bar{u}(x) v(x) \, \mathrm{d}x \quad \Rightarrow \quad \|u\|_2^2 = \langle u, u \rangle$$

The logarithmic norm of $\mathrm{d}^2/\mathrm{d}x^2$

Can we find a constant $\mu_2[\mathrm{d}^2/\mathrm{d}x^2]$ such that

$$\langle u, u'' \rangle \leq \mu_2[\mathrm{d}^2/\mathrm{d}x^2] \cdot \|u\|_2^2$$

for all functions $u \in C_0^2[0,1]$?

Yes and $\mu_2[\mathrm{d}^2/\mathrm{d}x^2] = -\pi^2$

Integration by parts

$$\int_0^1 uv' \, \mathrm{d}x = [uv]_0^1 - \int_0^1 u'v \, \mathrm{d}x$$

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

$$\langle u, v' \rangle = -\langle u', v \rangle$$

Apply to $\mathrm{d}^2/\mathrm{d}x^2 \quad \Rightarrow$

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

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 $\mathrm{d}^2/\mathrm{d}x^2$ 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* $\mathrm{d}^2/\mathrm{d}x^2$ *on* $C_0^2[0,1]$ *is*

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

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

$$\langle v, Au \rangle = v^{\mathrm{T}} A u = (A^{\mathrm{T}} v)^{\mathrm{T}} u = \langle A^* v, u \rangle$$

A^{T} is the adjoint of A

A matrix is self-adjoint ("symmetric") if $A = A^{\mathrm{T}}$

Self-adjoint differential operators . . .

Example $\mathrm{d}^2/\mathrm{d}x^2$ on $C_0^2[0,1]$

Integrate by parts

$$\langle v, u'' \rangle = -\langle v', u' \rangle = \langle v'', u \rangle$$

So $\mathrm{d}^2/\mathrm{d}x^2$ *is a self-adjoint operator*

More generally,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)$$

is self-adjoint on $C_0^2[0,1]$

Eigenvalues of self-adjoint operators . . .

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

$$\begin{aligned} \lambda\|u\|_2^2 &= \langle u, \lambda u\rangle = \langle u, Au\rangle = \langle A^* u, u\rangle \\ &= \langle Au, u\rangle = \langle \lambda u, u\rangle = \bar{\lambda}\|u\|_2^2 \end{aligned}$$

So $\lambda = \bar{\lambda}$ implies *real eigenvalues*

Eigenvectors of self-adjoint operators . . .

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

$$\begin{aligned} \lambda\langle v, u\rangle &= \langle v, Au\rangle = \langle A^* v, u\rangle \\ &= \langle Av, u\rangle = \mu\langle v, u\rangle \end{aligned}$$

So $(\lambda - \mu)\langle v, u\rangle = 0 \quad \Rightarrow \quad \langle v, u\rangle = 0$ implying that

eigenvectors are orthogonal

Elliptic operators

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

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

Example $-\mathrm{d}^2/\mathrm{d}x^2$ 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,

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

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 $-\mathrm{d}^2/\mathrm{d}x^2$ as $\mu_2[\mathrm{d}^2/\mathrm{d}x^2] = -\pi^2$ on $C_0^2[0,1]$

Negative Laplacian $-\Delta$ (leads to FEM theory)

8. From Finite Difference to Finite Element

Start with linear differential equation

$$\mathcal{A}u = f \qquad + \text{ boundary conditions}$$

Finite Difference Method (FDM). The main idea

Replace functions u and f by vectors and *differential operator $\mathcal{A}$ by matrix* to get a linear system of equations

Example

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}u = f(x) \quad \Rightarrow \quad T_{\Delta x}u = f$$

Finite Elements and the Galerkin method

Galerkin Method. The main idea

Approximate function u *by polynomial* and *keep differential operator* $\mathcal{A}$ *as is!*

Take some polynomial v satisfying boundary conditions. Insert into original equation to get $\mathcal{A}v \approx f$

Question Which polynomial gives the *best approximation*?

Answer *Choose* v *to minimize the residual* $\|\mathcal{A}v - f\|_2$

Best approximation = least squares

Let $\{\varphi_j\}$ be a polynomial basis, and make the *ansatz*

$$v(x) = \sum_{1}^{N} c_j \varphi_j(x)$$

Minimizing $\|\mathcal{A}v - f\|_2$ is equivalent to requiring that *the residual is orthogonal to each and every* φ_i

$$\langle \varphi_i, \mathcal{A}v - f \rangle = 0 \qquad \forall i$$

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

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

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

$$a_{ij} = \langle\varphi_i, \mathcal{A}\varphi_j\rangle \qquad\qquad b_i = \langle\varphi_i, f\rangle$$

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*

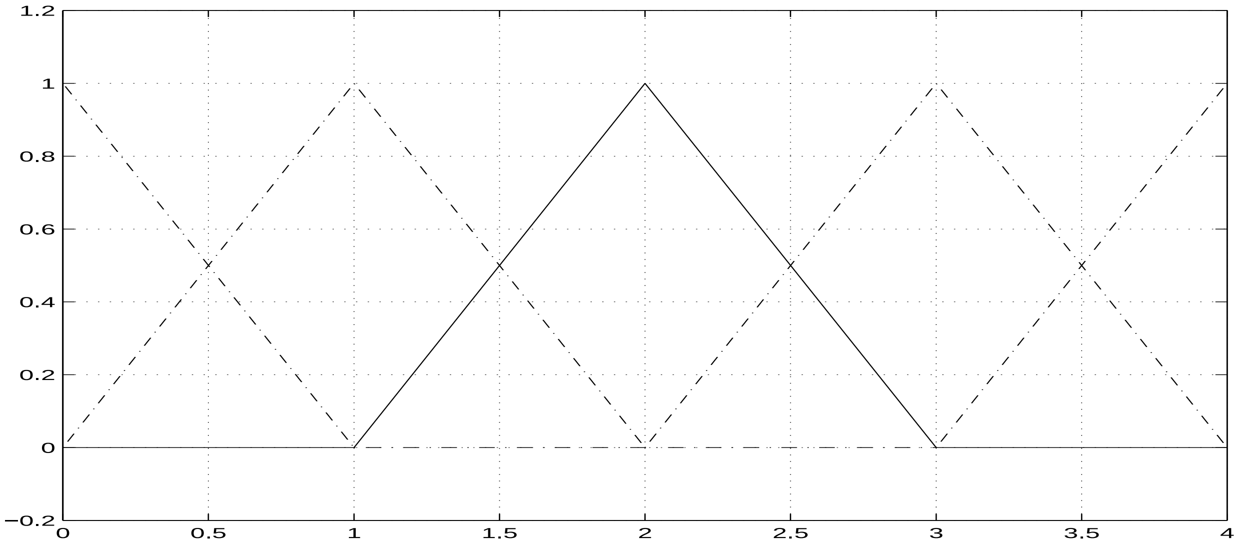
$$a(v,u) = \langle v, f \rangle$$

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 *piecewise linear basis polynomials*

$\varphi_j(x_i) = 1$ if $i = j$, otherwise 0



Piecewise linear interpolant $v \approx u$ can be written

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

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

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

which is equivalent to the *finite element equation* $Kc = b$

$$\sum_{j=1}^{N} \langle \varphi_i', \varphi_j'\rangle c_j = \langle \varphi_i, f\rangle \qquad \forall \varphi_i \in \mathcal{V}$$

The *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

Equation system

Assume an equidistant grid with spacing Δx. Note that

$$\begin{aligned} \varphi_i'(x) &= 1/\Delta x && \text{on} \quad [x_{i-1}, x_i] \\ \varphi_i'(x) &= -1/\Delta x && \text{on} \quad [x_i, x_{i+1}] \\ \varphi_i'(x) &= 0 && \text{elsewhere} \end{aligned}$$

Then

$$\langle \varphi_i', \varphi_i' \rangle = \int_{x_{i-1}}^{x_{i+1}} \frac{1}{\Delta x^2} \, \mathrm{d}x = \frac{2}{\Delta x}$$

$$\langle \varphi_i', \varphi_{i+1}' \rangle = \int_{x_i}^{x_{i+1}} \frac{-1}{\Delta x^2} \, \mathrm{d}x = \frac{-1}{\Delta x}$$

Stiffness matrix

For equidistant grid with spacing Δx the *stiffness matrix* is

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

Note

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

2) It is *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

$$\langle \varphi_i, f \rangle \approx \langle \varphi_i, \sum_0^N f_j \varphi_j \rangle = \sum_{k=-1}^{1} f_{i+k} \langle \varphi_i, \varphi_{i+k} \rangle$$

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

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 Δx the *mass matrix* is

$$B_{\Delta x} = \frac{\Delta x}{6} \, \mathrm{tridiag}(1 \quad 4 \quad 1)$$

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*

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

and *mass matrix*

$$B_{\Delta x} = \frac{\Delta x}{6}\, \mathrm{tridiag}(1 \quad 4 \quad 1)$$

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