Numerical Methods for Differential Equations

Chapter 3: FDM for 2p-BVPs and Sturm–Liouville

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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

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

Spatial symmetric 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 $\to$ finite differences $\to$ 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 $y' = \{y'(x_i)\}$

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

From derivatives to 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

From derivatives to matrices...

Central difference

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

Matrix representation

$$\begin{pmatrix} y_1' \\ y_2' \\ \vdots \\ y_N' \end{pmatrix} \approx \frac{1}{2\Delta x} \begin{pmatrix} -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{N+1} \end{pmatrix}$$

From derivatives to 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 now two-dimensional

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

From derivatives to 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 two solutions $\bar{y}_n = 1$ and $\tilde{y}_n = (-1)^n$

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 2D nullspace spanned by

$\bar{y} = (1 \quad 1 \ldots 1)^{\mathrm{T}}$ 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 two solutions $\bar{y}_n = 1$ and $\hat{y}_n = n$, respectively

This corresponds directly to $y = 1$ and $y = x$

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 $\Delta x = 1/(N+1)$

FDM discretization

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

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

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

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

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

A (nonlinear) system $F(y) = 0$ for N unknowns $y_1, y_2, \ldots, y_N$

Note how *boundary values* enter

3. Newton's method $F(y) = 0$

Let $y^{(k)}$ approximate the solution y and expand in Taylor series

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

Define $y^{(k+1)}$ by $\quad 0 =: F(y^{(k)}) + F'(y^{(k)}) \cdot (y^{(k+1)} - y^{(k)})$

Newton's method (mathematical formulation)

$$y^{(k+1)} := y^{(k)} - [F'(y^{(k)})]^{-1} F(y^{(k)})$$

Jacobian matrix $F'(y) = \{\partial F_i / \partial y_j\}$

For the FDM the 2p-BVP Jacobian matrix is

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

Tridiagonal matrix, with

- Super- and subdiagonal elements $1/\Delta x^2$
- Diagonal elements $-2/\Delta x^2 - \partial f / \partial y_i$
- Sparse LU decomposition runs in $\mathrm{O}(N)$ time
- Solution effort moderate even when N is large

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

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

Then convergence is quadratic

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

4. **Boundary conditions** come in many types

In many cases the problem is linear, but boundary conditions vary

- **Dirichlet conditions**

  $y(0) = \alpha\,; \quad y(1) = \beta$ straightforward to implement

- **Neumann conditions**

  $y'(0) = \gamma\,; \quad y(1) = \beta$ requires special attention

- **Robin conditions**

  $y(0) + c \cdot y'(0) = \kappa\,; \quad y(1) = \beta$ requires same attention

for the method's convergence order to be preserved

Neumann problem

Example
$$y'' = f(x, y)$$
$$y(0) = \alpha; \quad y'(1) = \beta$$

For second-order convergence, we must approximate also $y'(1)$ to second order

Standard symmetric approximation

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

requires points to the right of $x = 1$

What grid to use?

Neumann problem, approach 1

Example
$$y'' = f(x,y)$$
$$y(0) = \alpha; \quad y'(1) = \beta$$

Equidistant grid, $x_n = n\Delta x$ with $\Delta x = \frac{1}{N}$ and $x_{N+1} = 1 + \Delta x$

$$y'(1) = \beta \quad \to \quad \frac{y_{N+1} - y_{N-1}}{2\Delta x} = \beta$$

$\Rightarrow$ $y_{N+1} := 2\beta\,\Delta x + y_{N-1}$ is of second order at $x = 1$

Neumann problem, approach 2

Example
$$y'' = f(x, y)$$
$$y(0) = \alpha; \quad y'(1) = \beta$$

Equidistant grid, $x_n = n\Delta x$ with $\Delta x = \frac{1}{N+1/2}$ and

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

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

$\Rightarrow$ $y_{N+1} := \beta\,\Delta x + y_N$ is of second order at $x = 1$

Need to approximate $y(1) \approx \frac{y_N + y_{N+1}}{2}$

Neumann problem, approach 3

Example
$$y'' = f(x,y)$$
$$y(0) = \alpha; \quad y'(1) = \beta$$

Equidistant grid, $x_n = n\Delta x$ with $\Delta x = \frac{1}{N+1}$ and $x_{N+1} = 1$

$$y'(1) = \beta \quad \rightarrow \quad \frac{y_{N-1} - 4y_N + 3y_{N+1}}{2\Delta x} = \beta$$

$\Rightarrow$ $y_{N+1} := \frac{1}{3}\left(2\beta\Delta x + 4y_N - y_{N-1}\right)$ is of second order at $x = 1$

All three approaches work! It's a matter of taste.

Robin problem

Example

$$y'' = f(x, y)$$
$$y(0) = \alpha; \quad y(1) + cy'(1) = \kappa$$

Equidistant grid, with $x = 1$ between grid points

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

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

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

Other two approaches analogous

5. FDM on adaptive grids

Left and right divided differences

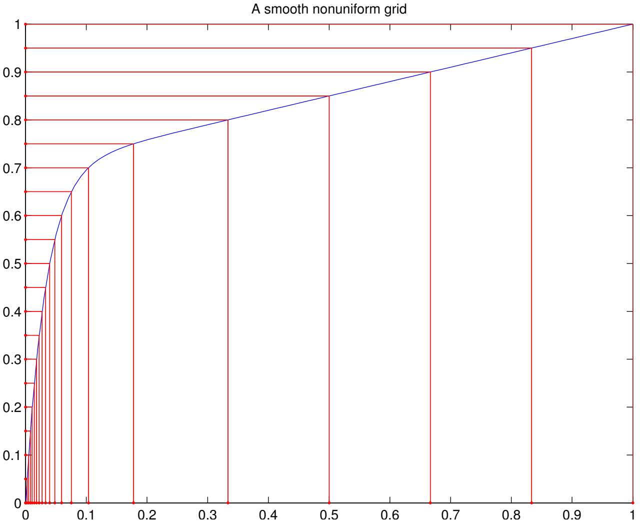
$$D^- y_i = \frac{y_i - y_{i-1}}{x_i - x_{i-1}} = \frac{y_i - y_{i-1}}{h^-} \qquad D^+ y_i = \frac{y_{i+1} - y_i}{x_{i+1} - x_i} = \frac{y_{i+1} - y_i}{h^+}$$

Then approximate derivatives by finite differences

$$y_i' \approx \frac{h^- D^+ y_i + h^+ D^- y_i}{h^+ + h^-}$$

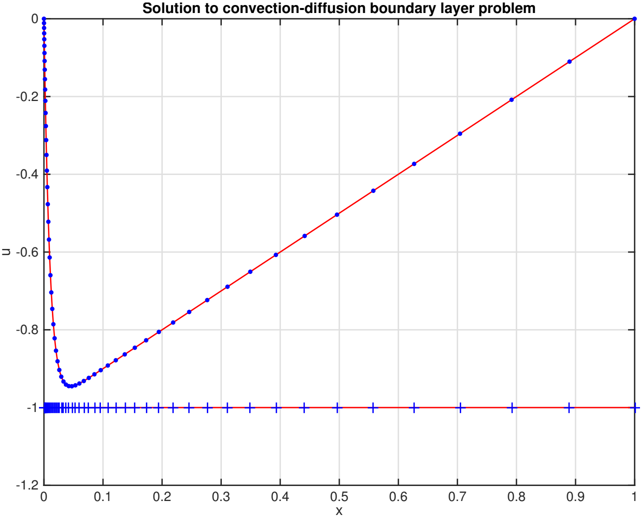
$$y_i'' \approx 2\,\frac{D^+ y_i - D^- y_i}{h^+ + h^-}$$

This is 2nd order only on *smooth grids* with $h^+/h^- = 1 + \mathrm{O}(N^{-1})$



A smooth nonuniform grid
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Adaptive grids $u'' + 100u' = 100$



6. Sturm–Liouville eigenvalue problems

Diffusion problem

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

Separation of variables (one space dimension)

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

Sturm–Liouville eigenvalue problem

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

Sturm–Liouville eigenvalue problems...

Wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}\,; \qquad u(t,a) = u(t,b) = 0$$

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

$$-\omega^2 y = c^2 y'' \qquad y(a) = y(b) = 0$$

Sturm–Liouville eigenvalue problem

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

Why Sturm–Liouville eigenvalue problems?

Öresund bridge

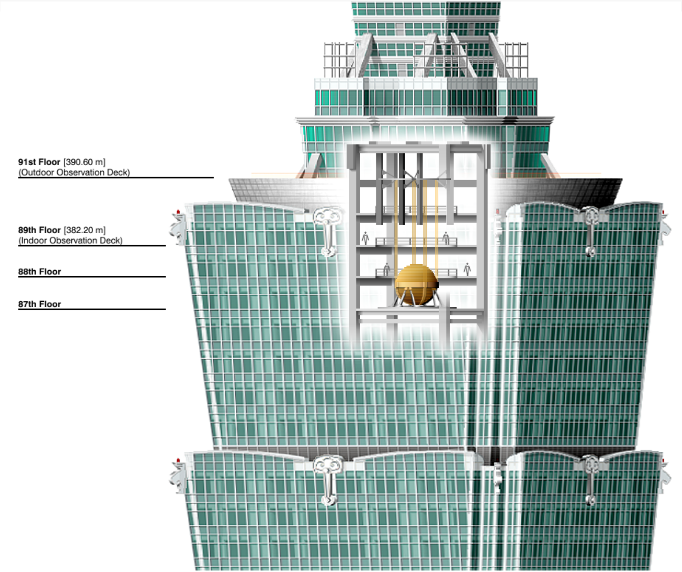
Fluid–structure interaction

Tacoma Narrows Bridge 1940

Tuned mass dampers

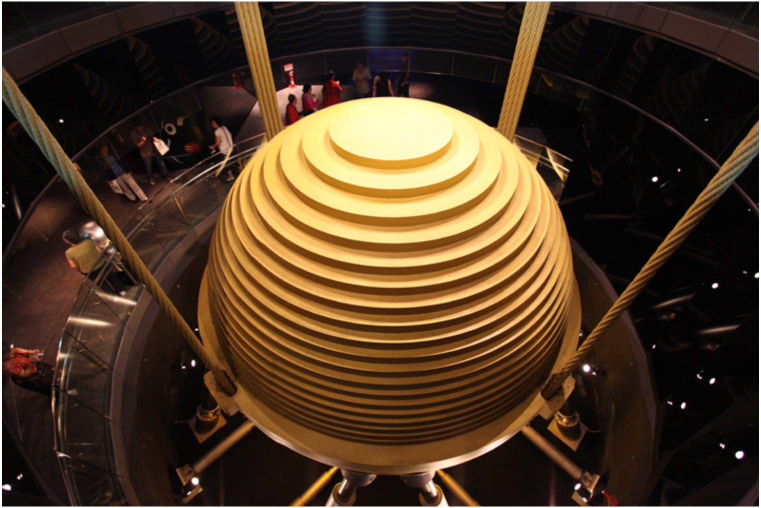
Stockbridge damper (1926) – anti-fatigue devices

Taipei 101



Somewhat larger tuned mass damper (660 000 kg)

It rocks



Gustaf Söderlind: *Mathematics rocks too!*

Music instruments

Compression loads, buckling and sun kinks

Quantum mechanics

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi$$

This is a Sturm–Liouville eigenvalue problem, with energy levels E_k defined by the eigenvalues

Sturm–Liouville eigenvalue problem

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

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

Discretization *Matrix eigenvalue problem*

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

Note Analytic eigenvalue problem converts to algebraic!

Symmetric discretizations

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\,\frac{\mathrm{d}y}{\mathrm{d}x}\right)\Big|_{x=x_i} \approx \frac{\big(p(x)y'(x)\big)\big|_{x_i+\frac{\Delta x}{2}} - \big(p(x)y'(x)\big)\big|_{x_i-\frac{\Delta x}{2}}}{\Delta x}$$

$$p(x_i + \frac{\Delta x}{2})\; y'(x)\big|_{x_i+\frac{\Delta x}{2}} \approx p\left(x_i + \frac{\Delta x}{2}\right)\frac{y(x_{i+1}) - y(x_i)}{\Delta x}$$

(similar for $x_i - \frac{\Delta x}{2}$) lead to

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

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

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

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

Symmetric tridiagonal $N \times N$ eigenvalue problem

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

There are N eigenvalues $\lambda_{\Delta x,n} = \lambda_n + O(\Delta x^2)$

Consider $y'' = \lambda y$ with boundary conditions $y(0) = y(1) = 0$

Analytic solution

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

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

Eigenvalues and eigenfunctions for $k = 1, 2, \ldots$

$$\begin{aligned} \lambda_k &= -(k\pi)^2 \\ y_k(x) &= \sin k\pi x \end{aligned}$$

Fourier modes (harmonic analysis) associated with $\mathrm{d}^2/\mathrm{d}x^2$

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 problem...

Algebraic eigenvalue problem

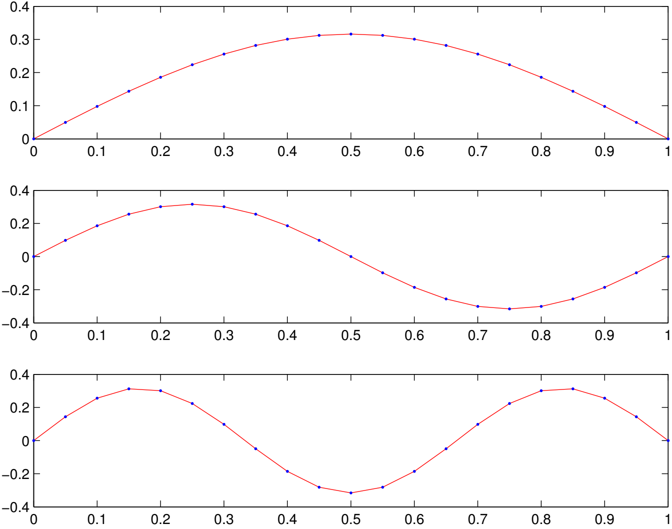
$$T_{\Delta x}\, y = \lambda_{\Delta x}\, y$$

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

Note There are only N discrete eigenvalues

First three eigenvectors of $T_{\Delta x}$ at $N = 19$



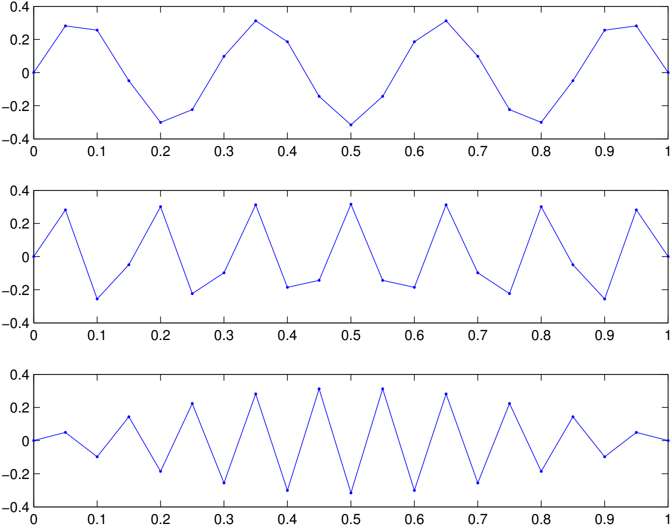
Discrete eigenvalues $\lambda_{\Delta x}$	-9.8493	-39.1548	-87.1948
Exact eigenvalues λ	-9.8696	-39.4784	-88.8264
Relative errors	0.21%	0.82%	1.84%

Note

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

  (Here approximately first 4 – 5 modes)

Eigenvectors 7, 13, 19 of $T_{\Delta x}$ at $N = 19$



7. 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 eigenvalues $\lambda[S]$, noting that the n^{th} equation of $Sy = \lambda y$ is

$$y_{n+1} + y_{n-1} = \lambda y_n$$

Eigenvalues and difference equations

Linear difference equation $y_{n+1} + y_{n-1} = \lambda y_n$ with boundary values $y_0 = 0 = y_{N+1}$

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

Two roots z and $1/z$ (product 1) implies general solution

$$y_n = Az^n + Bz^{-n}$$

Boundary condition $\quad y_0 = 0 = A + B \quad \Rightarrow \quad y_n = A(z^n - z^{-n})$

Eigenvalues and difference equations...

Boundary condition $y_{N+1} = 0 = A(z^{N+1} - z^{-(N+1)}) \quad \Rightarrow$

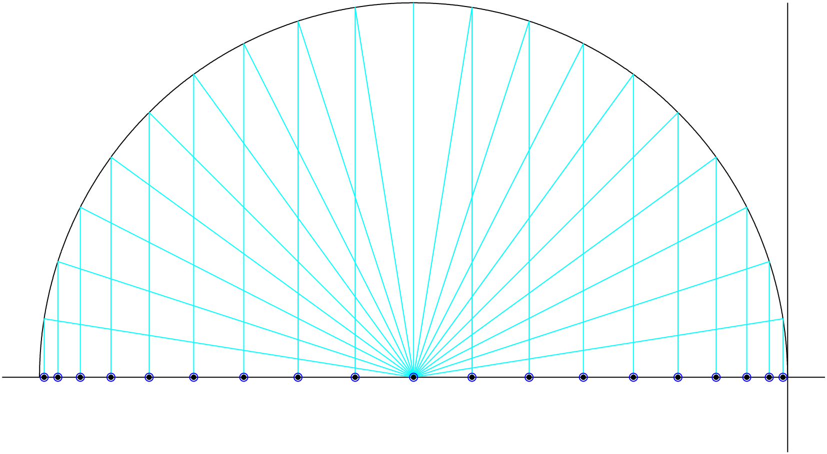
$$z^{2(N+1)} = 1 \quad \Rightarrow \quad z_k = \exp\left(\frac{k\pi \mathrm{i}}{N+1}\right) \qquad k = 1:N$$

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

$$\lambda_k[S] = z_k + 1/z_k = 2\cos\frac{k\pi}{N+1}$$

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 $T_{\Delta x} := T/\Delta x^2$ with $\Delta x = 1/(N+1)$ as an operator approximation

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

on $x \in [0,1]$

Corollary *The eigenvalues of $T_{\Delta x}$ are*

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

for $k \ll N$

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}x}\rho(x) = (2x^{\mathrm{T}} A^{\mathrm{T}} A x^{\mathrm{T}} x - 2x^{\mathrm{T}} x^{\mathrm{T}} A^{\mathrm{T}} A x)/(x^{\mathrm{T}} x)^2 := 0$$

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

So $\rho(x) = \lambda^2$, therefore $\|A\|_2 = \max|\lambda[A]|$ if $A^{\mathrm{T}} = A$

Proofs. Logarithmic norm

Definition (real A)

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

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

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

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

So $\rho(x) = \lambda$, therefore $\mu_2[A] = \max \lambda[A]$

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*

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

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 $\mu_2[T_{\Delta x}] \approx -\pi^2$ implies the existence of a *unique solution*, as

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

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

$$\|u\|_{L^2}^2 = \int_0^1 u(x)^2 \, \mathrm{d}x$$

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

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

Note For the operator norm, $\|T_{\Delta x}^{-1}\|_{\Delta x} \equiv \|T_{\Delta x}^{-1}\|_2$

8. Convergence of finite difference methods

Simplest model problem (1D Poisson equation)

$$y'' = f(x)$$
$$y(0) = \alpha; \quad y(1) = \beta$$

Equidistant discretization

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

Insert exact continuous 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 of local error, using $f(x_i) = y''(x_i)$

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

Only *even powers* of Δx due to *symmetry*. In particular, we get

$$\|l\|_{\Delta x} \leq \Delta x^2 \frac{1}{12} \max_{\xi \in [0,1]} |y^{(4)}(\xi)|$$

Definition *The global error is defined by* $e(x_i) = y_i - y(x_i)$

Convergence

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

$$\|e\|_{\Delta x} = c_1 \Delta x^2 + c_2 \Delta x^4 + \dots$$

Again only *even powers* due to *symmetry*

Convergence

Consider the problem $y'' = f$ discretized by 2nd order FDM

$$T_{\Delta x} u = f(x)$$

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

$$\begin{aligned} \textit{Numerical solution} \quad & T_{\Delta x} u = f(x) \\ \textit{Exact solution} \quad & T_{\Delta x} y(x) = f(x) - l(x) \\ \textit{Error equation} \quad & T_{\Delta x} e(x) = l(x) \end{aligned}$$

where $e(x) = u - y(x)$ is the *global error*

Convergence…

Solve $T_{\Delta x} u = f$ formally to get

$$\begin{aligned} \textit{Numerically} \quad & u = T_{\Delta x}^{-1} \cdot f(x) \\ \textit{Exact} \quad & y(x) = T_{\Delta x}^{-1} \cdot (f(x) - l(x)) \\ \textit{Global error} \quad & e(x) = T_{\Delta x}^{-1} \cdot l(x) \\ \textit{Error bound} \quad & \|e\|_{\Delta x} \leq \|T_{\Delta x}^{-1}\|_2 \cdot \|l\|_{\Delta x} \end{aligned}$$

Recall

- $\mu_2[T_{\Delta x}] \approx -\pi^2 \;\Rightarrow\; \|T_{\Delta x}^{-1}\|_2 \lessapprox 1/\pi^2$
- $\|e\|_{\Delta x} \leq \|T_{\Delta x}^{-1}\|_2 \cdot \|l\|_{\Delta x}$
- $\|l\|_{\Delta x} \leq \Delta x^2 \frac{1}{12} \max_{\xi\in[0,1]} |y^{(4)}(\xi)|$

We therefore have

$$\|e\|_{\Delta x} \leq C \cdot \|l\|_{\Delta x} = \frac{C}{12} \max_{\xi\in[0,1]} |y^{(4)}(\xi)| \Delta x^2$$

and we have convergence as $\Delta x \to 0$

The 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)

$$\textit{Consistency} + \textit{Stability} \Rightarrow \textit{Convergence}$$

"Fundamental theorem of numerical analysis"