Boundary value problems (BVP)

An IVP has the form $y'(t) = f(t, y(t))$, $y(0) = y_0$

- Causality: $y(t)$ depends only on $y(s)$, $s \leq t$
- One derivative $\Rightarrow$ one initial condition

A BVP has the form $\begin{cases} y''(x) = f(x, y(x)) \\ y(a) = \alpha, \quad y(b) = \beta \end{cases}$

- Spatial problem: $y(x)$ depends on y both to the right and left of x
- Two derivatives $\Rightarrow$ two boundary conditions

IVP strategy: time-step $y_n \rightarrow y_{n+1}$

BVP strategy: solve for $\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \approx \begin{bmatrix} y(x_1) \\ y(x_2) \\ \vdots \\ y(x_N) \end{bmatrix}$ all at once,

since the values all depend on each other

General idea :

diff. operator　　functions　　spatial variable

$$\left(\frac{d^2}{dx^2} y\right)(x) = f(x, y(x))$$

$$\Big\downarrow \text{ Discretize}$$

matrix

$$T\bar{y} = \bar{f}(\bar{x}, \bar{y})$$

vector $\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$　　vector $\begin{bmatrix} f(x_1, y_1) \\ \vdots \\ f(x_N, y_N) \end{bmatrix}$　　grid $\begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$

The right-hand-side part is obvious.

How do we do $\frac{d^2}{dx^2} \longrightarrow T$?

Back to Taylor series. Since

$$y(x+\Delta x) = y(x) + \Delta x\, y'(x) + \mathcal{O}(\Delta x^2),$$

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

This is a first-order forward difference approximation to $y'(x)$

$\mathcal{O}(\Delta x)$, will get back to how to def. orders for BVP setting

A backward difference approx. is

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

We can do better:

$$y(x+\Delta x) = y(x) + \Delta x\, y'(x) + \frac{\Delta x^2}{2} y''(x) + \mathcal{O}(\Delta x^3)$$

$$y(x-\Delta x) = y(x) - \Delta x\, y'(x) + \frac{\Delta x^2}{2} y''(x) + \mathcal{O}(\Delta x^3)$$

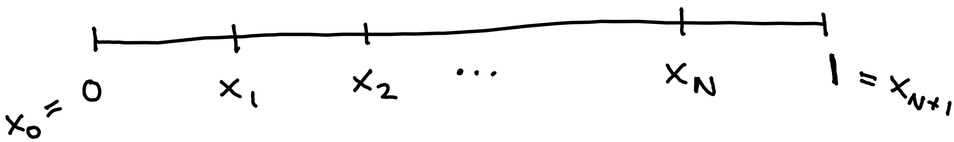
$$\Rightarrow \quad y'(x) = \frac{y(x+\Delta x) - y(x-\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Central (symmetric) difference, 2nd-order

Similarly (exercise!)

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

Now introduce a grid on $x \in [0,1]$



Uniform: $x_{k+1} = x_k + \Delta x$

N computational nodes: $x_1, \dots, x_N$

2 extra nodes: x_0, x_{N+1}

Suitable for boundary conditions $y(0) = \alpha$, $y(1) = \beta$

Other BC require other grids (later)

Then

$$y'(x) \approx \frac{y(x+\Delta x) - y(x)}{\Delta x} \Rightarrow y'(x_k) \approx \frac{y(x_{k+1}) - y(x_k)}{\Delta x}$$

Write this on matrix-vector form $\longrightarrow$

$$\underbrace{\begin{bmatrix} y'(x_1) \\ y'(x_2) \\ y'(x_3) \\ \vdots \\ y'(x_N) \end{bmatrix}}_{\in \mathbb{R}^N} \approx \frac{1}{\Delta x} \underbrace{\begin{bmatrix} -1 & 1 & 0 & & & \\ 0 & -1 & 1 & & & \\ 0 & 0 & -1 & 1 & & \\ & & & \ddots & \ddots & \\ & & & & -1 & 1 \\ & & & & 0 & -1 \end{bmatrix}}_{S_F \in \mathbb{R}^{N \times N}} \underbrace{\begin{bmatrix} y(x_1) \\ y(x_2) \\ y(x_3) \\ \vdots \\ y(x_N) \end{bmatrix}}_{\in \mathbb{R}^N} + \frac{1}{\Delta x} \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ y(x_{N+1}) \end{bmatrix}$$

$= y(1) = \beta$

Known from BC!

For backward diff. instead

$$\overline{(y')}(\bar{x}) \approx \frac{1}{\Delta x} \underbrace{\begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{bmatrix}}_{S_B} \bar{y}(x) + \frac{1}{\Delta x} \begin{bmatrix} -\alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Note that these matrices behave similarly to the diff. op.

$$y(x) \equiv 1 \quad \to \quad \bar{y} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \quad \text{and}$$

$$\frac{d}{dx} y = 0 \quad \text{while} \quad S_B \bar{y} + \frac{1}{\Delta x} \begin{bmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Central differences:

$$\overline{(y')}(\bar{x}) \approx \frac{1}{2\Delta x} \underbrace{\begin{bmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & & 0 & 1 \\ & & & & -1 & 0 \end{bmatrix}}_{S_{\Delta x}} \bar{y}(\bar{x}) + \frac{1}{2\Delta x} \begin{bmatrix} -\alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$$

and $\longrightarrow$

$$\overline{(y'')}(\bar{x}) \approx \underbrace{\frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}}_{T_{\Delta x}} \bar{y}(\bar{x}) + \frac{1}{\Delta x^2}\begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$$

Note:

$$y \equiv 1 \Rightarrow \frac{d^2}{dx^2} y \equiv 0 \quad \text{and} \quad T_{\Delta x}\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} + \frac{1}{\Delta x^2}\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$y(x) = x \Rightarrow \frac{d^2}{dx^2} y \equiv 0 \quad \text{and} \quad T_{\Delta x}\begin{bmatrix} 1 \\ 2 \\ \vdots \\ N \end{bmatrix} + \frac{1}{\Delta x^2}\begin{bmatrix} 0 \\ \vdots \\ 0 \\ N+1 \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

BVP FDM discretization

Summary

BVP: $\begin{cases} y''(x) = f(x, y(x)) \\ y(0) = \alpha \ , \ y(1) = \beta \end{cases}$

Grid: $x_k = k\Delta x \quad , \quad k = 1, \dots, N$

Approx.: $\bar{y} = [y_1, y_2, \dots, y_N]$

Discr. problem: $\begin{cases} \dfrac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} = f(x_i, y_i) \\ y_0 = \alpha \ , \ y_{N+1} = \beta \end{cases}$

Matrix-vector form: $T_{\Delta x}\bar{y} = \begin{bmatrix} f(x_1, y_1) \\ \vdots \\ f(x_N, y_N) \end{bmatrix} - \dfrac{1}{\Delta x^2}\begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$

Important: note that while $T_{\Delta x}\bar{y}$ is linear in $\bar{y}$, the whole problem is nonlinear due to the $f(x_i, y_i)$ terms.

We will consider how to solve such algebraic nonlinear equations later.

If $f(x, y(x)) = f(x)$ we have in fact a linear problem, which simplifies everything.

Other boundary conditions

So far we considered

Dirichlet conditions : $\boxed{y(a) = \alpha}$

German, "Dirikle"

There are also

Neumann conditions : $\boxed{y'(a) = \alpha}$

German, "Nojmann", not "Ne-u-mann"

and

Robin conditions : $\boxed{y(a) + c\,y'(a) = \alpha}$

French, "Ro-bang", not Swedish Robin

Always come in pairs :

E.g.

Homogeneous Dirichlet conditions $\Rightarrow$ $y(a) = 0$, $y(b) = 0$

Mixed Dirichlet and Neumann $\Rightarrow$ $y(a) = \alpha$, $y'(b) = \beta$

Dirichlet is straightforward, just replace

y_0 or y_{N+1} with the BC value

For Neumann/Robin, we must approximate

the $y'(a)$ using the available approx. $\{y_i\}$

If approx. of $\frac{d^2}{dx^2}$ is 2nd-order (as usual)

also BC approx. must be 2nd-order

Otherwise the full discr. is not 2nd-order!

Various approaches $\longrightarrow$

Problem: $\begin{cases} y''(x) = f(x, y(x)) \\ y(0) = \alpha \ , \ \underline{y'(1) = \beta} \end{cases}$

Neumann

Grid?

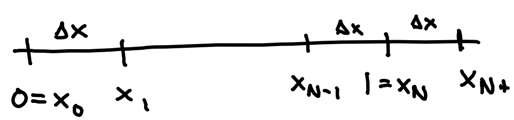
Standard 2nd-order central approximation

of y': $$y'(x) = \frac{y(x+\Delta x) - y(x-\Delta x)}{2\Delta x}$$

$\Rightarrow$ need points to left and right of $x=1$

Approach 1:

$\begin{cases} x_k = k\Delta x \\ \Delta x = \frac{1}{N} \end{cases}$



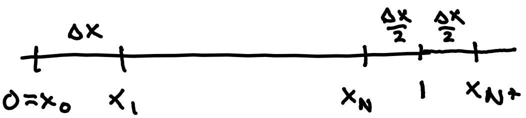
Discretize $y'(1) = \beta$ by $$\frac{y_{N+1} - y_{N-1}}{2\Delta x} = \beta$$

Replace y_{N+1} by $y_{N-1} + 2\Delta x\beta$ in all formulas where needed.

Approach 2:

If we don't want a node at $x=1$, maybe due to a singularity there

$$\begin{cases} x_k = k\Delta x \\ \Delta x = \dfrac{1}{N+1/2} \\ x_N = 1 - \dfrac{\Delta x}{2}, \quad x_{N+1} = 1 + \dfrac{\Delta x}{2} \end{cases}$$



Approx. $y'(1)=\beta$ by $\dfrac{y_{N+1} - y_N}{\Delta x} = \beta$

not N-1

$2 \cdot \frac{\Delta x}{2} = \Delta x$

No grid point at $x=1 \Rightarrow$ no direct approx. of $y(1)$

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

so $\dfrac{y_{N+1} + y_N}{2}$ is a 2nd-order approx.

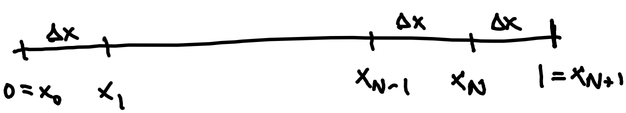
Approach 3:

No points at $x > 1$, maybe because problem undefined there. Can't use central approx. Instead:

$$y'(x) = \frac{y(x-2\Delta x) - 4y(x-\Delta x) + 3y(x)}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

exercise

$$\begin{cases} x_k = k\Delta x \\ \Delta x = \dfrac{1}{N+1} \end{cases}$$



Approx. $y'(1) = \beta$ by $\dfrac{y_{N-1} - 4y_N + 3y_{N+1}}{2\Delta x} = \beta$

Note:
- If the problem has no singularity, etc. either approach is fine. Just choose by taste.
- If the Neumann cond. is on the left, we need e.g. $x_k = (k-1)\Delta x$ or $(k-\frac{1}{2})\Delta x$.
- Robin BC analogous - issue is to approx y'.

Solving the discretized BVP

We saw that $y'' = f(x,y)$ + Dirichlet BC

becomes

$$T_{\Delta x}\,\bar{y} = \begin{bmatrix} f(x_1,y_1) \\ \vdots \\ f(x_N,y_N) \end{bmatrix} - \frac{1}{\Delta x^2}\begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$$

(Other BCs $\to$ similar equations.)

We can write this as $\boxed{F(\bar{y}) = 0}$

where $F : \mathbb{R}^N \to \mathbb{R}^N$ is given by

$$\begin{cases} F(\bar{y})_i = \dfrac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} - f(x_i,y_i), \quad i = 2,\dots,N-1 \\[2ex] F(\bar{y})_1 = \dfrac{\alpha - 2y_1 + y_2}{\Delta x^2} - f(x_1,y_1) \\[2ex] F(\bar{y})_N = \dfrac{y_{N-1} - 2y_N + \beta}{\Delta x^2} - f(x_N,y_N) \end{cases}$$

Sometimes we write $F_i(\bar{y})$ instead of $F(\bar{y})_i$

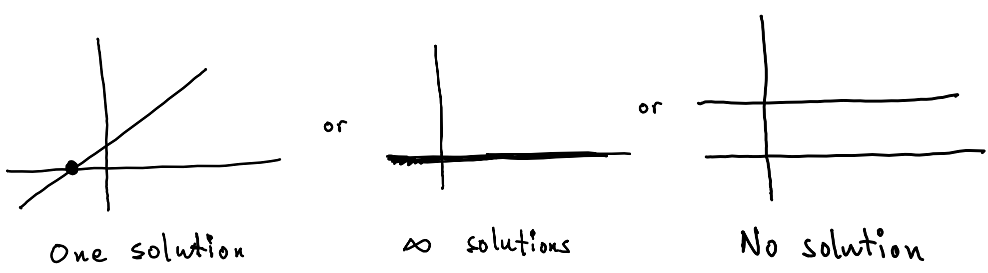
but it must <u>not</u> be $F(y_i)$.

$y_i \in \mathbb{R}$ but F takes $\mathbb{R}^N$-arguments.

How do we solve $F(y) = 0$?

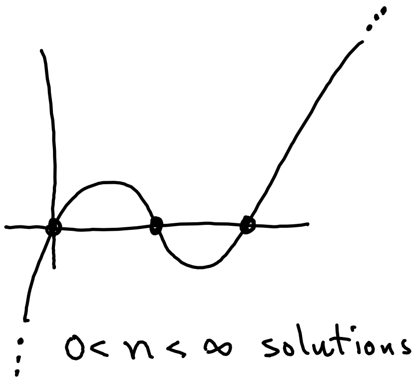
Big field, many methods - can only give limited view here

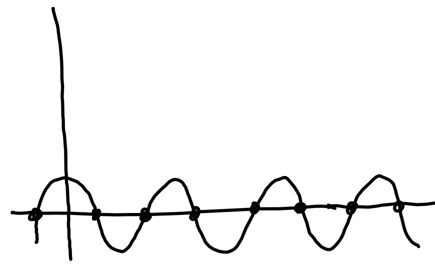
If F linear:



Easy to determine which, and to solve (if possible).

If F nonlinear, also:





$\Rightarrow$ Can only expect <u>local</u> convergence to

to closest <u>local zero x^*</u>, in general

(But our problems will typically have unique solutions.)

$\longrightarrow$

General approach : iterative method

$$x^1 \to x^2 \to \cdots \to x^k \to x^{k+1},$$

better and better approx. to x^*.

Method converges if error $e^k = x^k - x^* \to 0$ as $k \to \infty$.

- If $\|e^{k+1}\| \le c\|e^k\|$, $0<c<1$,

  we have linear convergence

- If $\|e^{k+1}\| \le c\|e^k\|^2$, $0<c<1$,

  we have quadratic convergence

Note that this is a different type of convergence than the convergence $\|u_n - u(t_n)\| \leq Ch^p$ that we consider for time-stepping methods.

Note also that "Quadratic >> Linear"

Ex. $c = \frac{1}{2}$, $e_1 = \frac{1}{2}$:

	Linear	Quadratic
e_2	$1/4$	$1/8$
e_3	$1/8$	$1/128$
e_4	$1/16$	$1/32768$
e_5	$1/32$	$\sim 4.6 \cdot 10^{-10}$
e_6	$1/64$	Accurate to machine precision

A linearly convergent method is given by the fixed point iteration:

$$x^{k+1} = x^k + F(x^k)$$

Usually written $x^{k+1} = g(x^k)$ with $g(x) = x + F(x)$ where x^* is a fixed point of g if $x^* = g(x^*)$.

Very useful for analysis, but too slow in practice.

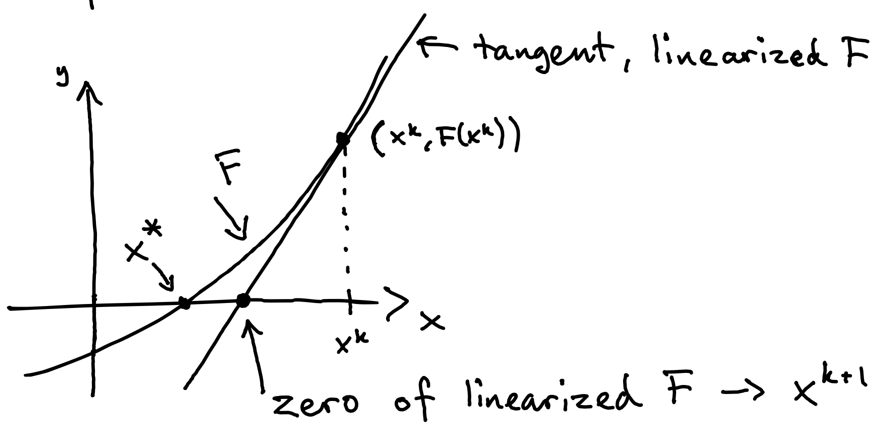
A (locally) quadratically convergent method is Newton's method:

$$F'(x^k)(x^{k+1} - x^k) = -F(x^k).$$

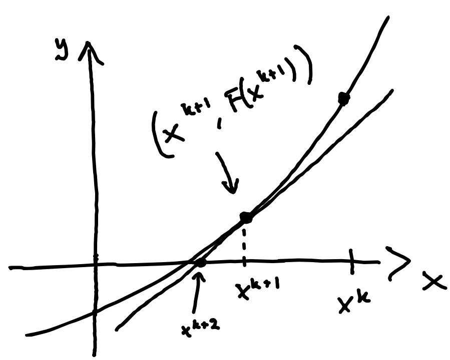
Let's see how to arrive at this method. →

Idea: linear equations are easy to solve, so <u>linearize</u> repeatedly, at the points $(x^k, F(x^k))$

Step k:



Step k+1:



x^{k+2} already very close to x^*!

Equation for tangent: ("$y - y_0 = k(x - x_0)$")

$$y - F(x^k) = F'(x^k) \cdot (x - x^k)$$

At the zero, $y = 0$, so we choose x^{k+1} by

$$-F(x^k) = F'(x^k)(x^{k+1} - x^k)$$

The above was for $F : \mathbb{R} \to \mathbb{R}$.

If $F : \mathbb{R}^N \to \mathbb{R}^N$, we linearize by neglecting higher-order terms in a Taylor expansion around x^k:

$$F(x) = F(x^k + (x - x^k))$$

$$= F(x^k) + F'(x^k) \cdot (x - x^k) + \cancel{h.o.t.}$$

$\Rightarrow$ same formula, but what is F'?

Def. The Jacobian matrix of $F: \mathbb{R}^N \to \mathbb{R}^N$ is $F' \in \mathbb{R}^{N \times N}$ with

$$(F')_{i,j} = \frac{\partial F_i}{\partial x_j} .$$

$\Rightarrow$ The j:th column of $F'(x)$ is $F(x)$ differentiated with respect to x_j

---

It can be shown that Newton's method is quadratically convergent, if $x^0 - x^*$ is small enough. No practical estimate for how small is small enough...

Heuristics $\longrightarrow$

- If F comes from an IE step $y_{n+1} = y_n + hf(y_{n+1})$ then y_n is usually a good starting guess

- If F comes from $y'' = f(y)$, $y(0) = \alpha$, $y(1) = \beta$, then the linear function $y(x) = \alpha + (\beta - \alpha)x$ could be a better guess than e.g. $y(x) \equiv 0$.

- Modern software has lots of features that can improve convergence success rate and speed, e.g. line-search, preconditioners, etc.

- A typical very common reason for why Newton does not converge is that F' is incorrect

In BVP $\longrightarrow$

Our discretization of the BVP

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

is $F(\bar{y}) = 0$ with $\bar{y} = [y_1, \dots, y_N]^T$ and

$$F(\bar{y}) = T_{\Delta x}\,\bar{y} + \frac{1}{\Delta x}\begin{bmatrix}\alpha \\ 0 \\ \vdots \\ 0 \\ \beta\end{bmatrix} - \begin{bmatrix} f(x_1, y_1) \\ \vdots \\ f(x_N, y_N)\end{bmatrix}$$

$$\Rightarrow F'(\bar{y}) = T_{\Delta x} - \operatorname{diag}\left(\begin{bmatrix} f_y'(x_1, y_1) \\ \vdots \\ f_y'(x_N, y_N)\end{bmatrix}\right)$$

Exercise: verify this via

$$(F'(\bar{y}))_{i,j} = \frac{\partial (F(\bar{y}))_i}{\partial y_j}$$

Sometimes written

$$F'(\bar{y}) = \text{tridiag}\left(\frac{1}{\Delta x^2} \, , \, -\frac{2}{\Delta x^2} - f'_y(x_i, y_i) \, , \, \frac{1}{\Delta x^2} \right)$$

1st subdiagonal (constant elements) — main diagonal (i:th element) — 1st superdiagonal (constant elements)

Since F' is tri-diagonal,

- it is very <u>sparse</u> (lots of zeroes)
  $\Rightarrow$ low storage requirements

- solving $(F'(\bar{y}))z = b$ is very efficient, $\mathcal{O}(N)$ rather than $\mathcal{O}(N^3)$ for a general matrix.

Sturm-Liouville eigenvalue problems

Ubiquitous problem type that we can solve with our BVP techniques:

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

not necessarily differentiable

both unknown

Motivation 1

From simple diffusion problem (week 5):

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

Separation of variables (actually useful, sometimes!):

$$u(t,x) = y(x)\,v(t) \Rightarrow y\dot{v} = (py'v)' = (py')'v$$

$$\Rightarrow \frac{\dot{v}}{v} = \frac{(py')'}{y} = \lambda \text{ because eq. holds } \forall t \text{ and } \forall x$$

constant

and dep. only on t, dep. only on x

$\Rightarrow$ S-L problem $\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) = \lambda y$ for y

and $v(t) = e^{\lambda t} v(0)$.

Motivation 2 (similar)

From wave equation (week 6):

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

Suppose $u(t,x) = e^{i\omega t} y(x)$, $\quad y(a) = y(b) = 0$.

oscillation fixed shape

Then

$$-\omega^2 \cancel{e^{i\omega t}} y(x) = c^2 \cancel{e^{i\omega t}} y''(x)$$

$\therefore$ S-L problem $y'' = \lambda y$ with $\lambda = \frac{-\omega^2}{c^2}$

So we can use S-L problems as a tool to solve more complex problems.

Motivation n

[Series of applications in mechanics and other areas where S-L eigenvalue problems feature prominently.]

Approximation

usually infinitely many

Exact problem: Find eigenvalues λ and eigenfunctions y such that

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

Discretization: Find N eigenvalues λ_j and eigenvectors $y^j \in \mathbb{R}^N$, $j = 1, \dots, N$, such that

$$T y^j = \lambda_j y^j.$$

$T \in \mathbb{R}^{N\times N}$ discretization of $\frac{d}{dx}\left(p\frac{d}{dx}\,\cdot\right) + q\,\cdot$ with hom. Dirichlet BC

Analytic eigenvalue problem $\rightarrow$ algebraic eigenvalue problem

If p differentiable: $p'y' + py''$

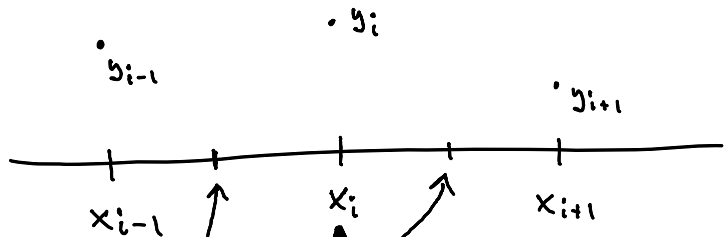
$\to$ discretize y' and y'' as usual

Assume p not differentiable

Common strategy (also elsewhere):

Two steps - first outer derivative, then inner

Grid:



Extra help nodes where no y-approx. is stored; $x_i - \frac{\Delta x}{2}$, $x_i + \frac{\Delta x}{2}$

Want approx. to $\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)$ here

$$\left.\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)\right|_{x=x_i} \overset{\text{outer}}{\approx} \frac{\left.\left(p(x)y'(x)\right)\right|_{x=x_i+\frac{\Delta x}{2}} - \left.\left(p(x)y'(x)\right)\right|_{x=x_i-\frac{\Delta x}{2}}}{\Delta x}$$

and

$$\left.\left(p(x)y'(x)\right)\right|_{x=x_i+\frac{\Delta x}{2}} \overset{\text{inner}}{\approx} p\left(x_i+\frac{\Delta x}{2}\right)\frac{y(x_{i+1}) - y(x_i)}{\Delta x}$$

$\longrightarrow$

Similarly, $(p(x)y'(x))_{x_i - \frac{\Delta x}{2}} \approx p(x_i - \frac{\Delta x}{2}) \dfrac{y_i - y_{i-1}}{\Delta x}$

In total, with $p_{i\pm\frac{1}{2}} = p(x_i \pm \frac{\Delta x}{2})$,

$$\begin{cases} \dfrac{p_{i-\frac{1}{2}} y_{i-1} - (p_{i-\frac{1}{2}} + p_{i+\frac{1}{2}}) y_i + p_{i+\frac{1}{2}} y_{i+1}}{\Delta x^2} + q(x_i) y_i = \lambda_{\Delta x} y_i \\ y_0 = y_{N+1} = 0 \end{cases}$$

Note that there are N solution pairs $(\lambda_{\Delta x}^j, y_{\Delta x}^j)$

Both $\lambda_{\Delta x}^j$ and $y_{\Delta x}^j$ depend on $\Delta x = \frac{1}{N+1}$.

Can write it on matrix form:

$$\operatorname{tridiag}\left(\frac{p_{i-\frac{1}{2}}}{\Delta x^2}, -\frac{p_{i-\frac{1}{2}} + p_{i+\frac{1}{2}}}{\Delta x^2} + q(x_i), \frac{p_{i+\frac{1}{2}}}{\Delta x^2} \right) y_{\Delta x}^j = \lambda_{\Delta x}^j y_{\Delta x}^j$$

Note that we get the standard central discretization of y'' when $p(x) \equiv 1$ and $q(x) \equiv 0$, since $p_{i \pm \frac{1}{2}} = 1$, $q_i = 0$ $\forall i$.

Let's use this as a benchmark problem:

$$\begin{cases} y'' = \lambda y \\ y(0) = y(1) = 0 \end{cases} \longrightarrow \begin{cases} \dfrac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} = \lambda_{\Delta x}\, y \\ y_0 = y_{N+1} = 0, \quad \Delta x = \dfrac{1}{N+1} \end{cases} \qquad (y = y_{\Delta x})$$

Exact solution? General form

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

A, B constants

Boundary conditions:

$$y(0) = 0 \Rightarrow B = 0$$

$$y(1) = 0 \Rightarrow \underline{A = 0} \quad \text{or} \quad \sqrt{-\lambda} = k\pi, \quad k = 1, 2, \ldots$$

$\Rightarrow y \equiv 0$, not eigenvector $\qquad$ ($k = 0$ also $\Rightarrow y = 0$)

$\boxed{\begin{array}{l}\textbf{Theorem: } \text{The eigenvalues and eigenfunctions of } \dfrac{d^2}{dx^2} \text{ are} \\ \lambda_k = -k^2\pi^2 \quad \text{and} \quad y^k(x) = \sin(k\pi x)\end{array}}$

[Numerical test comparing the algebraic eigenvalues and eigenvectors $\lambda_{\Delta x, j}$ and $y^j_{\Delta x}$ satisfying $T_{\Delta x}\, y^j_{\Delta x} = \lambda_{\Delta x, j}\, y^j_{\Delta x}$ to the exact λ_j, y^j.]

We have $\lambda_{\Delta x, j} = -j^2\pi^2 + \mathcal{O}(\Delta x^2)$,

but the constant in $\mathcal{O}(\Delta x^2)$ grows with j

$\Rightarrow$ "good" approximation for $\sim \sqrt{N}$ smallest (in magnitude) eigenvalues

$\dfrac{d^2}{dx^2}$ is an important operator and its discretization

$T_{\Delta x} = \dfrac{1}{\Delta x^2}\, \text{tridiag}(1, -2, 1)$ is an important matrix

Let's find some more properties of such matrices $\rightarrow$

Symmetric, tridiagonal Toeplitz matrices

<u>Def.</u> A Toeplitz matrix is constant along diagonals.

(Like $T_{\Delta x}$.)

Typically arise when discretizing differential operators.

Much research on e.g. eigenvalue distributions, norms, inverses, etc. Can solve $Tx = b$ in $O(N^2)$ rather than $O(N^3)$.

(like $T_{\Delta x}$)

When <u>symmetric</u> and <u>tridiagonal</u>, we have an explicit formula for the eigenvalues and eigenvectors, which will also give us e.g. the norm of the matrix.

Let's find these for $T_{\Delta x}$: (With the ultimate aim of using it for some error analysis.)

Note that $\lambda[cI + A] = c + \lambda[A]$

$\left(\text{but } \lambda[A+B] \neq \lambda[A] + \lambda[B] \text{ in general!}\right)$

and $\lambda[cA] = c\lambda[A]$, $c \in \mathbb{R}$.

$$\Rightarrow \lambda[T_{\Delta x}] = \frac{1}{\Delta x^2}\left(-2 + \lambda[S]\right)$$

where

$$S = \begin{bmatrix} 0 & 1 & 0 & \cdots & & 0 \\ 1 & 0 & 1 & & & \\ 0 & 1 & 0 & \ddots & & \\ & & \ddots & & & \\ & & & & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}.$$

$Sy = \lambda y$ means $\begin{cases} y_{i+1} + y_{i-1} = \lambda y_i \\ y_0 = y_{N+1} = 0 \end{cases}$

Linear difference equation!

Char. eq.: $z^2 - \lambda z + 1 = 0$

Trick: If z_1 and z_2 are two roots, then

$$(z-z_1)(z-z_2) = 0$$

$$z^2 - (z_1+z_2)z + z_1 z_2 = z^2 - \lambda z + 1$$

$\Rightarrow$ $\underbrace{z_1 + z_2 = \lambda}_{①}$ and $\underbrace{z_1 z_2 = 1}_{②}$

$\Rightarrow$ General solution $y_n = A z_1^n + B z_2^n$

$$\overset{②}{=} A z_1^n + B z_1^{-n}$$

BC $y_0 = 0 \Rightarrow 0 = A + B \Rightarrow y_n = A(z_1^n - z_1^{-n})$

[Where are we going? Want to compute $\lambda = z_1 + z_2$,
i.e. find all possible (z_1, z_2).]

$\longrightarrow$

The 2nd BC $y_{N+1} = 0$

$$\Rightarrow \quad 0 = A\left(z_1^{N+1} - z_1^{-N-1}\right)$$

$$\Rightarrow \quad z_1^{2(N+1)} = 1 \qquad \left(\begin{array}{l} A=0 \Rightarrow y=0, \\ \text{not eigenvector} \end{array}\right)$$

$$\Rightarrow \quad z_1 = e^{\frac{k\pi i}{N+1}} \quad , \quad k = 1, \ldots, N.$$

(Not $k=0$, as then $z_1 = 1 \Rightarrow z_2 = 1 \Rightarrow$ double root $\Rightarrow y_n = A \cdot 1^n + B \cdot n \cdot 1^n$ which cannot satisfy the BC unless $A=B=0$.)

$$\therefore \quad \lambda = z_1 + z_2 = z_1 + z_1^{-1} =$$

1

$$= \cos\left(\tfrac{k\pi}{N+1}\right) + i\sin\left(\tfrac{k\pi}{N+1}\right) + \cos\left(-\tfrac{k\pi}{N+1}\right) + i\sin\left(-\tfrac{k\pi}{N+1}\right)$$

$$= 2\cos\left(\frac{k\pi}{N+1}\right) \quad , \quad k = 1, \ldots, N$$

This was for S. For $T_{\Delta x}$:

$$\lambda\left[T_{\Delta x}\right] = \frac{1}{\Delta x^2}\left(-2 + \lambda[S]\right) = \ldots \longrightarrow$$

[After some easy trigonometry involving $\cos(2x) = 1 - 2\sin^2 x$:]

Theorem The eigenvalues of the central FDM approximation $T_{\Delta x} \in \mathbb{R}^{N \times N}$ to $\frac{d^2}{dx^2}$ are

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

Note 1: $\sin x \approx x$ for small x

$$\Rightarrow \lambda_1[T_{\Delta x}] \approx -4(N+1)^2 \frac{\pi^2}{2^2(N+1)^2} = \underbrace{-\pi^2}$$

= smallest eigenvalue of $\frac{d^2}{dx^2}$

Note 2: $k = N \Rightarrow \sin\left(\frac{N\pi}{2(N+1)}\right) \approx 1$

$$\Rightarrow \lambda_N[T_{\Delta x}] \approx -4(N+1)^2$$

$\to -\infty$ as $N \to \infty$. This makes sense, as $\frac{d^2}{dx^2}$ has arbitrarily negative eigenvalues $-k^2\pi^2$

So why did we do all this?

1. To show that $T_{\Delta x}$ and $\frac{d^2}{dx^2}$ have similar properties

2. To compute $\|T_{\Delta x}\|$ and $\|T_{\Delta x}^{-1}\|$, to use in BVP error analysis.

<u>Def.</u> A matrix $A \in \mathbb{C}^{N \times N}$ is <u>normal</u> if

$$A^* A = A A^* .$$

<u>Theorem</u>: Every symmetric matrix $A \in \mathbb{R}^{N \times N}$ is normal.

<u>Theorem:</u> For a normal matrix A with eigenvalues λ_k, we have

$$\boxed{\|A\|_2 = \max_k |\lambda_k| .}$$

Proof omitted, because it does not contribute much to this course, see old slides if interested.

$\boxed{\begin{array}{l} \underline{\text{Corollary}} \\ \text{We have} \\ \qquad \|T_{\Delta x}\|_2 \approx 4(N+1)^2 \\ \text{and} \\ \qquad \|T_{\Delta x}^{-1}\|_2 \approx \frac{1}{\pi^2}. \end{array}}$

<u>Proof of the 2nd assertion:</u>

$\lambda_k(T_{\Delta x}) < 0$ (strictly) $\forall k \Rightarrow T_{\Delta x}^{-1}$ exists

and

$$\|T_{\Delta x}^{-1}\|_2 = \max_k \frac{1}{|\lambda_k(T_{\Delta x})|} = \frac{1}{|\lambda_1(T_{\Delta x})|} \approx \frac{1}{\pi^2}. \qquad \square$$

$$\left(\text{Since } Ax = \lambda x \Rightarrow x = A^{-1}\lambda x = \lambda A^{-1}x \Leftrightarrow A^{-1}x = \frac{1}{\lambda}x. \right)$$

Note: $\|T_{\Delta x}\|$ very large, $\|T_{\Delta x}^{-1}\|$ moderate size

"Differentiation bad" vs. "Integration good".

We will generalize this to operators and discuss e.g. $u_{xx} = f$ in Chapter 4.

$\longrightarrow$

Convergence of FDM for BVP

We consider only one problem and discr., but the approach is general.

$$\begin{cases} y'' = f(x,y) \\ y(0) = \alpha, \ y(1) = \beta \end{cases} \longrightarrow \begin{cases} \dfrac{y_{i-1} - 2y_i + y_{i+1}}{\Delta x^2} = f(x_i, y_i), \ i = 1, \dots, N \\ y_0 = \alpha, \ y_{N+1} = \beta \end{cases}$$

Local error: insert exact sol. into scheme

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

local error, ℓ function of x

Taylor expand $y(x_i - \Delta x)$ and $y(x_i + \Delta x)$ around x_i:

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

(Odd powers disappear due to symmetry.)

Let $\bar{\ell} = [\ell(x_0), \ell(x_1), \dots, \ell(x_N)]^T$. Then

$\uparrow = 0$, but include anyway so the numbering works out

$$\|\bar{\ell}\|_2 = \sqrt{\sum_{k=0}^{N} \ell(x_k)^2} \leq \sqrt{(N+1)\cdot \frac{2}{4!} \max_i \left(y^{(4)}(x_i)\right)^2 \Delta x^4 + \mathcal{O}(\Delta x^6)}$$

$$\leq C\sqrt{N+1}\,\Delta x^2 + \mathcal{O}(\Delta x^3)$$ where $C \in \mathbb{R}$ depends on $y^{(4)}$.

Note $\Delta x = \frac{1}{N+1}$ so $\sqrt{N+1} = \sqrt{\Delta x^{-1}} = \Delta x^{-1/2}$

and $\|\bar{\ell}\|_2 = \mathcal{O}(\Delta x^{3/2})$.

Makes more sense to measure in RMS-norm (Root-Mean-Square):

Similar conclusions can be drawn by using $\|\bar{\ell}\|_\infty$. $\|\cdot\|_{RMS}$ ~ average error $\|\cdot\|_\infty$ ~ max error. Important part is to compensate for different N.

$$\|\bar{\ell}\|_{RMS} = \sqrt{\sum_{k=0}^{N} \ell(x_k)^2 \cdot \Delta x} = \sqrt{\Delta x}\cdot \|\bar{\ell}\|_2$$

This discrete norm mimics the function norm

$$\|\ell\|_{L^2} = \sqrt{\int_0^1 \ell(x)^2\,dx}$$

If $u(x) \equiv 1$ with discr. $\bar{u} = [1, 1, \dots, 1]^T \in \mathbb{R}^N$

then $\|u\|_{L^2} = \sqrt{\int_0^1 1\,dx} = 1$ and

$$\|\bar{u}\|_2 = \sqrt{\sum_0^N 1^2} = \sqrt{N+1} \to \infty \quad \text{as } N \to \infty$$

$$\|\bar{u}\|_{RMS} = \frac{1}{\sqrt{N+1}} \|\bar{u}\|_2 = 1$$

$\therefore$ $\|\cdot\|_{RMS}$ is the proper norm to use for the discretized functions

It compensates for having more and more components in the vector.

We now have

$$\|\bar{e}\|_{RMS} = \mathcal{O}(\Delta x^2)$$

<u>Def.</u> The <u>order of consistency</u> of a FDM method for a BVP is p if the local error ℓ satisfies $\|\bar{\ell}\|_{RMS} = \mathcal{O}(\Delta x^p)$.

Note difference to ODE: p instead of $p+1$

Def. The <u>global error</u> is the function e that satisfies $e(x_i) = y_i - y(x_i)$

Def. The method is convergent of order p if

$$\|e(\bar{x})\|_{RMS} = \left\| [e(x_1), \dots, e(x_N)]^T \right\|_{RMS} = \mathcal{O}(\Delta x^p).$$

Theorem

Our central FDM discretization is of order 2 when applied to the linear problem $y''(x) = f(x)$.

Proof: With the grid $\bar{x} = [x_1, \dots, x_N]$, use the notation $u(\bar{x}) = \begin{bmatrix} u(x_1) \\ \vdots \\ u(x_N) \end{bmatrix}$ for a general function u.

Then $y(\bar{x})$ is the exact solution on the grid and $\bar{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$ is the approximation.

$\Longrightarrow$

We have

$$T_{\Delta x}\, \bar{y} = f(\bar{x}) \qquad \text{for approx. sol. } \bar{y}$$

$$T_{\Delta x}\, y(\bar{x}) = f(\bar{x}) - \ell(\bar{x}) \qquad \text{for exact sol } y(x)$$

$$\Rightarrow \quad T_{\Delta x}\, e(\bar{x}) = T_{\Delta x}\left(\bar{y} - y(\bar{x})\right)$$

$$= \ell(\bar{x})$$

Error equation : relation between local and global error.

$$\Rightarrow \quad e(\bar{x}) = T_{\Delta x}^{-1}\, \ell(\bar{x})$$

Matrix norm, $\|A\|_{RMS} = \|A\|_2$. Why?

$$\text{so} \quad \|e(\bar{x})\|_{RMS} \le \underbrace{\|T_{\Delta x}^{-1}\|_{RMS}}_{\approx \frac{1}{\pi^2}}\ \underbrace{\|\ell(\bar{x})\|_{RMS}}_{O(\Delta x^2)}$$

∴ The method is convergent of order 2. □

[What about $y'' = f(x,y)$? See p. 48.]

This procedure exemplifies the "meta-theorem"

Lax principle

$$\text{Consistency} + \text{Stability} = \text{Convergence}$$

Sometimes called "the fundamental theorem of numerical analysis".

Here:

Consistency : local error $\ell \to 0$ as $\Delta x \to 0$

Stability : $\| T_{\Delta x}^{-1} \| \leq C$ as $\Delta x \to 0$

$\Rightarrow$ Convergence: global error $e \to 0$ as $\Delta x \to 0$.

What about the nonlinear case

$$y''(x) = f(x, y(x)) \,?$$

Then we need to know that f has some good properties. The previous approach becomes

$$T_{\Delta x}\,\bar{y} = f(\bar{x}, \bar{y}) \qquad \text{for approx.}$$

$$T_{\Delta x}\,y(\bar{x}) = f(\bar{x}, y(\bar{x})) - \ell(\bar{x}) \qquad \text{for exact sol.}$$

and thus

no longer cancels

$$e(x) = T_{\Delta x}^{-1}\Big(\ell(\bar{x}) + f(\bar{x}, \bar{y}) - f(\bar{x}, y(\bar{x}))\Big)$$

By the triangle inequality we get

$$\|e(x)\| \le \|T_{\Delta x}^{-1}\|\Big(\|\ell(\bar{x})\| + \|f(\bar{x}, \bar{y}) - f(\bar{x}, y(\bar{x}))\|\Big)$$

$\longrightarrow$

e.g.

If f is Lipschitz continuous in the second variable with Lipschitz constant L then

$$\|f(\bar{x},\bar{y}) - f(\bar{x}, y(\bar{x}))\| \leq L\|\bar{y} - y(\bar{x})\|$$
$$= L\|e(x)\|$$

Hence, using $\|T_{\Delta x}^{-1}\| \leq \frac{1}{\pi^2}$,

$$\left(1 - \frac{L}{\pi^2}\right)\|e(x)\| \leq \frac{1}{\pi^2}\|\ell(\bar{x})\|$$

so that

$$\|e(\bar{x})\| = \mathcal{O}(\Delta x^2)$$

if $L \leq \pi^2$.

Alternatively, if we know the derivatives of f, we could expand in Taylor series like

$$f(\bar{x},\bar{y}) - f(\bar{x},y(\bar{x})) = f(\bar{x}, y(\bar{x}) + e(\bar{x})) - f(\bar{x}, y(\bar{x}))$$
$$= f_y'(\bar{x}, y(\bar{x}))\, e(\bar{x}) + \text{h.o.t.}$$

$\longrightarrow$

The higher-order terms (h.o.t.) would consist of tensor operations on multiple instances of $e(\bar{x})$. So while something can be done, it is not perfectly straight-forward.

$$\boxed{\text{In the nonlinear case, the specific properties of the nonlinearity always matter for the end result.}}$$