1 a

Model 1

stationary model

$$\begin{cases} u''(x) + \lambda e^{u(x)} = 0 \\ u(0)=0,\ u(1)=0 \end{cases},\ \lambda \in \mathbb{R}$$

properties:

1) $\lambda < 0 \Rightarrow \begin{cases} \exists!\ u(x) \quad (<0\ \forall x \in (0,1)) \\ \exists!\ \text{minimum at } x = 1/2 \end{cases}$

2) $\lambda > \lambda^*$: no (!) solution exists

3) $\lambda = \lambda^*$: one solution

4) $0 \le \lambda < \lambda^*$: two (!) solutions $\begin{cases} u_1(x) > 0 \\ u_2(x) > 0 \end{cases}$

both with a single maximum at $x = 1/2$

---

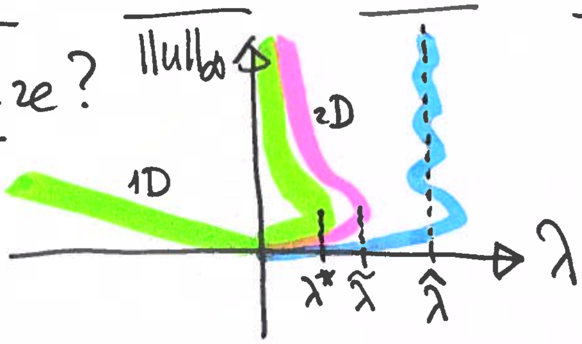
extensions

→ 2D : $\Delta u + \lambda e^u = 0 \quad (u(x,y) = \dots)$
$(x,y) \in [0,1] \times [0,1]$
$\sim$ 1D $\quad \tilde{\lambda}$ instead of λ^*

→ 3D : completely different!
at $\lambda = \hat{\lambda}$: ∞-many solutions

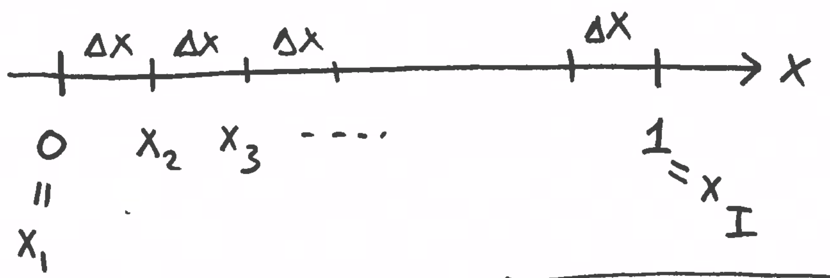
→ replace e^u by $\begin{cases} 1 + u + \frac{u^2}{2} + \frac{u^3}{6} : \infty\text{-many solutions} \\ 1 + u + \frac{u^2}{2} + \frac{u^3}{6} + \frac{u^4}{24} : \sim e^u\text{-case.} \end{cases}$

How to visualize?



$\|u\|_\infty = \max_{x \in [0,1]} |u(x)|$

1 b How to find the solutions?



$$\begin{cases} x_1 = 0 = 0 \cdot \Delta x \\ x_2 = \Delta x = 1 \cdot \Delta x \\ x_3 = 2\Delta x \\ \vdots \\ x_I = (I-1)\Delta x = 1 \end{cases}$$

!

$$\begin{cases} \text{FOR-loop} \\ x(i) = (i-1)\Delta x, \; i = 1, \dots, I \end{cases}$$

$$\Delta x = \frac{1}{I-1}$$

$$\boxed{u_1 = 0 \;, \; u_I = 0}$$

$\boxed{u_i : \text{approximation of } u(x) \text{ at } x = x_i}$

$u_2, u_3, \dots, u_{I-1}$ from:

$$u''\Big|_{x=x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + \mathcal{O}\left((\Delta x)^2\right)$$

$i = 2, 3, \dots, I-2, I-1$

Taylor:

$$\begin{cases} u_{i+1} = u_i + \Delta x\, u' + \frac{(\Delta x)^2}{2} u'' + \frac{(\Delta x)^3}{6} u''' + \frac{(\Delta x)^4}{24} u'''' + \dots \\ u_i = 1 \cdot u_i + \Delta x \cdot 0 + \frac{(\Delta x)^2}{2} 0 + 0 + 0 \dots \\ u_{i-1} = u_i + (-\Delta x) u' + \frac{(-\Delta x)^2}{2} u'' + \frac{(-\Delta x)^3}{6} u''' \dots \end{cases}$$

$$u''\Big|_{x=x_i} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

Define: $\vec{u} = \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ \vdots \\ u_{I-1} \end{pmatrix}$ and $D_2 = \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \Theta \\ & 1 & -2 & 1 & \\ & & & \ddots & \\ \Theta & & & & \\ & & & 1 & -2 \end{pmatrix}$

$(I-2) \times (I-2)$ matrix

1 c

$$\Rightarrow \boxed{D_2 \vec{u} + \lambda e^{\vec{u}} = \vec{0}}$$

componentwise

a nonlinear system.

How to solve?

re-write: $\vec{F}(\vec{u}) = \vec{0}$

choose Δx, or I

→ Newton-Raphson in $I-1$ dimensions

or alternative iterative methods to improve the efficiency ..

→ fsolve in Matlab

↦ define $\vec{F}$ in Matlab

and choose an appropriate initial guess

u_2

u_3

⋮

u_{I-1}

u_1 and u_I already given $(=0)$

$\Rightarrow$ plot (x , u_{plot})

with u(1) and u(2)

2

Model 2

(Linear PDE)

$$\frac{\partial u}{\partial t} = \kappa \cdot \frac{\partial^2 u}{\partial x^2}$$

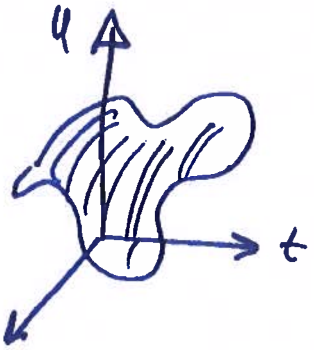
heat equation
(diffusion equation)

partial derivatives

P. D. E.
partial differential equation

$u(x,t) = ?$
temperature

$\kappa > 0$: conduction coefficient
(diffusion " ")



space $x \in [0,1]$ ← special case

time $t \in [0,T]$ ← given (final time)

IC: $u(x,0) = u_0(x) = \sin(\pi x)$
initial condition — given — special case

BCs : $u(0,t) = 0$, $u(1,t) = 0$
boundary conditions — special case

theory
$\Rightarrow u(x,t) = e^{-\pi^2 t} \sin(\pi x)$

Numerical solutions with Matlab:

"Method-of-lines" (two steps: first space x, then time t)

1) a "uniform grid"

Δx Δx Δx ...

(SPACE) x

$x_1 = 0$ x_2 x_3 x_4 ... $1 = x_I$ ← final index

$$\boxed{\begin{array}{l} x_i = (i-1)\Delta x \\ i = 1, 2, 3, \dots, I \end{array}}$$

$x_1 = 0$, $x_2 = \Delta x$
... $x_I = (I-1)\Delta x$

3

$$\Rightarrow \quad i=I: \ (I-1)\Delta x = x_I = 1$$

$$\Rightarrow \boxed{\Delta x = \frac{1}{I-1}}$$

choose one of the two

1b) approximate $\frac{\partial^2 u}{\partial x^2}$ at $x = x_i$:

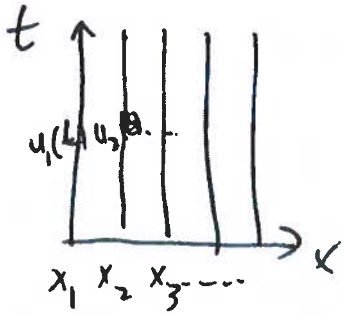
$$\frac{\partial^2 u}{\partial x^2}(x_i,t) \approx \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}$$

follows from Taylor expansions (see: "Numerieke Wiskunde" / numerical analysis course) $\Big\}$ error: $O((\Delta x)^2)$

with $u_i(t) \approx u(x_i,t)$

exact value at discrete x_i's and continuous t

1c) Define
$$\boxed{\vec{u}(t) \stackrel{def}{=} \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_{I-1}(t) \end{pmatrix}} \approx \begin{pmatrix} u(x_1,t) \\ u(x_2,t) \\ \vdots \\ u(x_{I-1},t) \end{pmatrix}$$



$$\Rightarrow \frac{\partial u}{\partial t}(x_i,t) \approx \frac{d}{dt}(u_i(t)) = \dot{u}_i(t)$$

$$\Longrightarrow \frac{d\vec{u}}{dt}(t) = \underbrace{\frac{1}{(\Delta x)^2}\begin{pmatrix} \ddots & \ddots & & 0 \\ & 1 \ \ -2 \ \ 1 & & \\ 0 & & \ddots & \ddots \end{pmatrix}}_{\text{call matrix } D_2} \vec{u}(t)$$

(tri-diagonal with eigenvalues: $\boxed{\lambda_i = \frac{-4}{(\Delta x)^2}\sin^2\left(\frac{\pi i \Delta x}{2}\right) \in \mathbb{R}^-}$)

and more to the left for smaller Δx

$$\begin{cases}
\dot{u}_1 = 0 & , \ u_1(0) = \sin(\pi x_1) = \sin(0) = 0 \\
\dot{u}_2 = \frac{u_3 - 2u_2 + u_1}{(\Delta x)^2} & , \ u_2(0) = \sin(\pi x_2) \\
\dot{u}_3 = \frac{u_4 - 2u_3 + u_2}{(\Delta x)^2} & , \ u_3(0) = \sin(\pi x_3) \\
\vdots & \vdots \\
\dot{u}_{I-1} = \frac{u_I - 2u_{I-1} + u_{I-2}}{(\Delta x)^2} & , \ u_{I-1}(0) = \sin(\pi x_{I-1}) \\
\dot{u}_I = 0 & , \ u_I(0) = \sin(\pi x_I) = \sin(\pi) = 0
\end{cases}$$

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1d) BCs: $\begin{cases} u_0 = 0 \\ u_I = 0 \end{cases}$ $\rightsquigarrow$ can be used in the first row and last row of the matrix D_2

IC: $\vec{u}(0) = \begin{pmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \sin(\pi x_I) \end{pmatrix} \overset{\text{def}}{=} \vec{u}_0$

$\Rightarrow$ ODE system: $\begin{cases} \dot{\vec{u}}(t) = D_2 \vec{u}(t) \\ \vec{u}(0) = \vec{u}_0 \end{cases}$ known

ordinary

solution

$$\vec{u}(t) = e^{tD_2}\vec{u}_0$$

in Matlab: "expm"

---

2) Euler-Forward (Explicit Euler) "EF"

note that matlab does not have zero-index $\rightarrow$ re-write starting from index 1

explicit: $\dfrac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = D_2 \vec{u}^n$ time step.

$n = 0, 1, 2, \dots, N$ ~ $t=0$ ~ $t=T$

time points: $t^n = (n-1)\Delta t$, $n = 1, \dots, N$

$t^N = T = (N-1)\Delta t$

$\boxed{\Delta t = \dfrac{T}{N-1}}$ given

choose one of the two

$$\vec{u}^{n+1} = (I + \Delta t D_2)\vec{u}^n$$

or

Euler-Backward (implicit Euler) "EB"

implicit: $\dfrac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = D_2 \vec{u}^{n+1} \Rightarrow \underbrace{(I - \Delta t D_2)}_{A}\vec{u}^{n+1} = \vec{u}^n$

in Matlab: "$\vec{u}^{n+1} = A \backslash \vec{u}^n$"

for loop in n-index

4a

(in)stability of EF (EB)

$$\begin{cases} y' = \lambda y \\ y(0) = y_0 \end{cases}$$

$\lambda \in \mathbb{C}$

$Re(\lambda) < 0$

"eigenvalue of system"

EF: $y_{n+1} = (1 + \lambda \Delta t) y_n$

EB: $y_{n+1} = \dfrac{1}{1 - \lambda \Delta t} y_n$

$Re(\lambda) < 0$

$|1 + \lambda \Delta t| < 1$, then stable

otherwise unstable

$\left| \dfrac{1}{1 - \lambda \Delta t} \right| < 1$ always stable ($Re(\lambda) < 0$)

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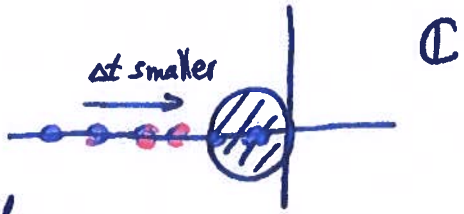
property of EF : numerically stable solutions, if $\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$

for higher resolution in space we need small Δx and, therefore, Δt "quadratically" smaller (expensive)

eigenvalues of D_2 lie in a unit circle :



property of EB :
numerically stable solutions for all $\Delta t > 0$!
BUT, we need to solve a linear system to obtain $\vec{u}^{n+1}$ from $\vec{u}^{n}$
at t^{n+1} at t^{n}

Note: the accuracy in space of EF $\approx$ EB

$\boxed{\text{Model 3}}$

$$\frac{\partial u}{\partial t} = d \cdot \frac{\partial^2 u}{\partial x^2} + \gamma\, u(1-u)$$

$d > 0$; nonlinear term ; "Fisher PDE" (population dynamics)

follow recipe in Model 2 :

$$\Rightarrow \quad \dot{\vec{u}}(t) = d\, D_2\, \vec{u}(t) + \vec{f}(\vec{u}(t))$$

$$\vec{f} = \begin{pmatrix} \gamma u_1(1-u_1) \\ \gamma u_2(1-u_2) \\ \vdots \\ \gamma u_{I-1}(1-u_{I-1}) \end{pmatrix}$$

check what would happen, if

2 EB is applied
(--- $\Rightarrow$ solve huge nonlinear system at each step $t^n \to t^{n+1}$)

1 EF : $\frac{\vec{u}^{n+1} - \vec{u}^{n}}{\Delta t} = d\, D_2\, \vec{u}^{n} + \vec{f}^{n} \Rightarrow \vec{u}^{n+1} = (I + d\Delta t D_2)\vec{u}^{n} + \Delta t \vec{f}^{n}$

loop in index n
($n \neq 0$!!)

6

find a "mix" between EF and EB:

not always stable (see heat equation) — EF

always stable but "expensive" — EB

$\rightsquigarrow$ IMEX method

IM = implicit (EB)

EX = explicit (EF)

$$\Rightarrow \quad \frac{\vec{u}^{n+1}-\vec{u}^{n}}{\Delta t} = d\, D_2\, \vec{u}^{n+1} + \vec{f}(\vec{u}^{n})$$

$$\Rightarrow \quad \vec{u}^{n+1}-\vec{u}^{n} = d\,\Delta t\, D_2\, \vec{u}^{n+1} + \Delta t\, \vec{f}(\vec{u}^{n})$$

not to forget!

$$\Rightarrow \quad \underbrace{(I - d\,\Delta t\, D_2)}_{\substack{\text{known matrix} \\ \text{call: } A}}\vec{u}^{n+1} = \underbrace{\vec{u}^{n} + \Delta t\, \vec{f}(\vec{u}^{n})}_{\substack{\text{known from previous step} \\ \text{call: } \vec{g}(\vec{u}^{n})}}$$

$\vec{u}^{n+1}$: to be determined for $n = 0, 1, 2, \ldots, N-1$

$$\Rightarrow \quad \boxed{A\, \vec{u}^{n+1} = \vec{g}(\vec{u}^{n})}$$

a linear system

" $\vec{u}^{n+1} = A \backslash \vec{g}^{n}$ "

Model 3

$$u_t = d u_{xx} + \left(\frac{u^2}{2}\right)_x + \tau u_{xxt} \quad \text{(from geohydrology)}$$

u_t: short notation for $\frac{\partial u}{\partial t}$

u_{xx}: $\frac{\partial^2 u}{\partial x^2}$

$(\;)_x$: $\frac{\partial}{\partial x}(\;)$

u_{xxt}: $\frac{\partial^3}{\partial x^2 \partial t}$

one-phase: "water"

non-monotone waves ("fingers")

$d > 0, \; \tau \geq 0$

two-phase: water - oil
or
water - oxygen
or
--

$$\frac{u^2}{u^2 + M(1-u)^2}$$

$$M = \frac{\mu_w}{\mu_o}$$ ← viscosity

7

Method-of-lines ("M.o.L."):

$$\dot{\vec{u}}(t) = d\, D_2 \vec{u}(t) + \vec{h}(\vec{u}(t)) + \tau D_2 \dot{\vec{u}}(t)$$

$$(I - \tau D_2)\dot{\vec{u}}(t) = d D_2 \vec{u}(t) + \vec{h}(\vec{u}(t))$$

call: M (matrix)

2 IMEX

$$M \frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = d D_2 \vec{u}^{n+1} + \vec{h}(\vec{u}^n)$$

$$\Rightarrow M(\vec{u}^{n+1} - \vec{u}^n) = d \Delta t D_2 \vec{u}^{n+1} + \Delta t \vec{h}(\vec{u}^n)$$

$$\Rightarrow \underbrace{(M - d\Delta t D_2)}_{\text{call: } B \text{ (matrix)}} \vec{u}^{n+1} = \underbrace{M\vec{u}^n + \Delta t \vec{h}(\vec{u}^n)}_{\text{call: } \vec{k}(\vec{u}^n)}$$

$$\Rightarrow \boxed{B\vec{u}^{n+1} = \vec{k}(\vec{u}^n)}$$

$$\vec{u}^{n+1} = B \backslash \vec{k}^n$$

at $x = x_i$: $\left(\frac{u^2}{2}\right)_x \approx \frac{u_{i+1}^2 - u_{i-1}^2}{4\Delta x}$

(comes from: $u_x \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$

Taylor (num. analysis) central finite differences

$$\vec{h}(\vec{u}(t)) = \begin{pmatrix} \frac{u_2^2 - u_0^2}{4\Delta x} \\ \frac{u_3^2 - u_1^2}{4\Delta x} \\ \vdots \end{pmatrix} \quad u_0^2 = 0$$

check final term

1 EF: $\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = d D_2 \vec{u}^n + \vec{h}^n + \tau D_2 \frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t}$

$$\underbrace{(I - \tau D_2)}_{=M}\vec{u}^{n+1} = \underbrace{(I + d\Delta t D_2 - \tau D_2)}_{=B}\vec{u}^n$$

$\vec{u}^{n+1} = M \backslash (B\vec{u}^n)$ loop in index n