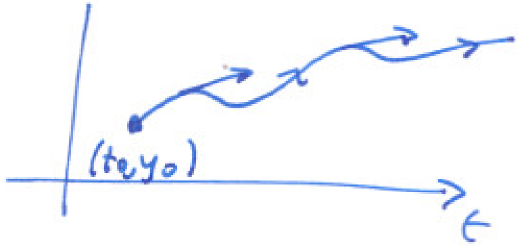
Numerical Methods for solving ODEs as initial value problems (IVPs)

Approximate a solution to



$$\frac{dy}{dt}(t) = f(y(t), t) \quad \text{for } t \geq t_0, \; y(t_0) = y_0$$

with $y \in \mathbb{R}^d$, $f : \mathbb{R}^d \times [t_0, \infty) \to \mathbb{R}^d$

Existence & uniqueness of a solution:

<u>Thm</u> Let f be defined and continuous on the strip $S = \{(y, t) \mid a \leq t \leq b, \; y \in \mathbb{R}^d\}$ w. a & $b < \infty$. Let there be a constant λ s.t.

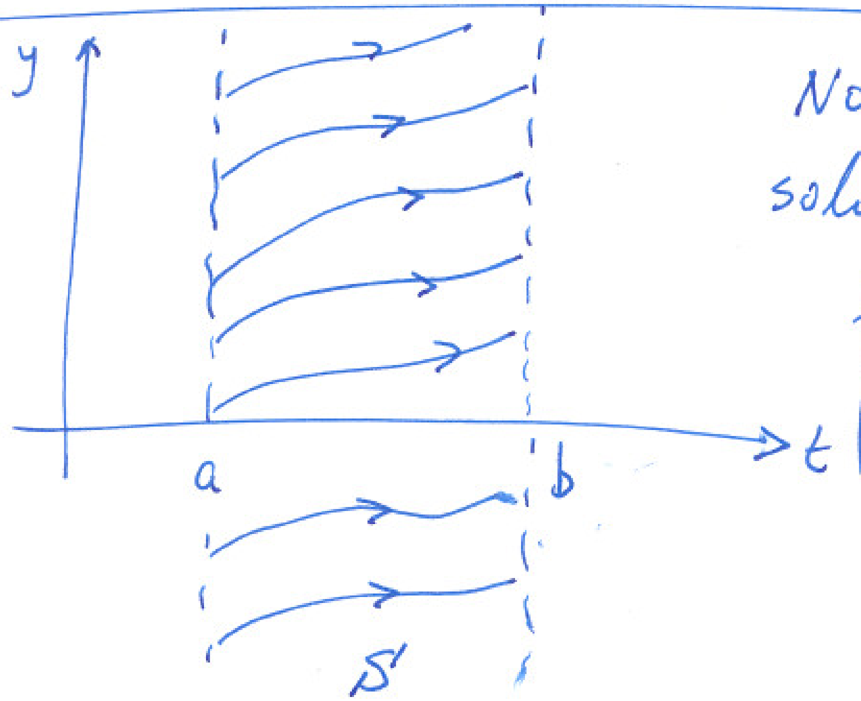
$$\| f(x, t) - f(y, t) \| \leq \lambda \| x - y \| \quad \left(\begin{array}{c}\text{Lipschitz} \\ \text{condition}\end{array}\right)$$

$\forall \; t \in [a, b]$ & all $x, y \in \mathbb{R}^d$. Then, for each $(y_0, t_0) \in S$, there exists a unique fn $y(t)$ satisfying:

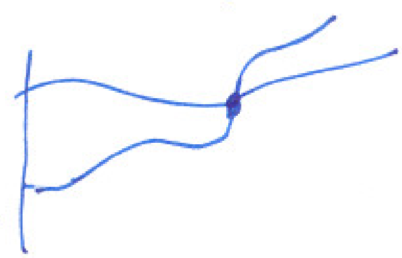
(i) $y(t)$ is continuously differentiable for $t \in [a,b]$

(ii) $\dfrac{dy}{dt} = f(y(t), t)$ for $t \in [a,b]$

(iii) $y(t_0) = y_0$



No crossing of solutions!



The Lipschitz condition is satisfied if

$\dfrac{\partial f_i}{\partial y_j}$, $i,j = 1,\dots,d$ exist on S', & are cont.

& bded there. Usually ~~not the case~~ only f is continuously diff. on S', but $\nabla_y f$ is not bded.

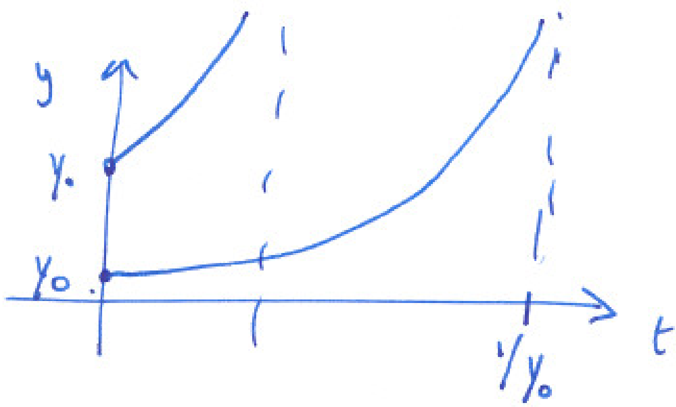
~~Ex:~~ $\cancel{\dfrac{dy}{dt} = y^2}$ ~~if~~ $\cancel{y(0) = 1 \Rightarrow y(t) = \dfrac{1}{1-t}}$

<u>Example</u> $\quad \dfrac{dy}{dt} = y^2 \; ; \; y(t_0) = y_0 \; ;$ No Lipschitz bd for all y.

$$\Rightarrow \quad y(t) = \frac{y_0}{1 - y_0(t - t_0)}$$

set $\begin{cases} t_0 = 0 \\ y_0 > 0 \end{cases}$. Solution diverges at $\bar{t} = \dfrac{1}{y_0}$

$$y(t) = \frac{y_0}{1 - y_0 t}$$



The solution to an IVP depends continuously upon its initial data:

<u>Thm</u>
Let $f : S' \to \mathbb{R}^d$ be continuous on

$S' = \{(y, t) \mid a \le t \le b, \; y \in \mathbb{R}^d\}$ & satisfy the Lipschitz ~~inequa~~ condition with constant λ.

Then, for ~~the~~ solutions $y(t; y_0)$ w. $y(t_0; y_0) = y_0$

$$\| y(t; y_1) - y(t; y_2) \| \le e^{\lambda(t - t_0)} \| y_1 - y_2 \|$$

Pf. $y(t;y_0) = y_0 + \int_{t_0}^{t} ds\, f(y(s;y_0),s) \quad t \geq t_0$

$\Rightarrow \|y(t;y_1) - y(t;y_2)\|$

$\leq \|y_1 - y_2\| + \int_{t_0}^{t} ds\, \|f(y(s;y_1),s) - f(y(s;y_2),s)\|$

$\leq \|y_1 - y_2\| + \lambda \int_{t_0}^{t} ds\, \|y(s;y_1) - y(s;y_2)\|$

Let $\Phi(t) = \int_{t_0}^{t} \|y(s;y_1) - y(s;y_2)\| ds \; ; \; t \geq t_0$

Note: $\Phi(t_0) = 0$.

$\Rightarrow \Phi'(t) - \lambda \Phi(t) \leq \|y_1 - y_2\|$

$\Rightarrow \underbrace{e^{-\lambda t}\Phi' - e^{-\lambda t}\lambda\Phi}_{= \frac{d}{dt}\left(e^{-\lambda t}\Phi\right)} \leq e^{-\lambda t}\|y_1 - y_2\|$; Integrate the ineq:

$e^{-\lambda t}\Phi(t) \leq -\frac{1}{\lambda}\left(e^{-\lambda t} - e^{-\lambda t_0}\right)\|y_1 - y_2\|$

$\Rightarrow \Phi(t) \leq -\frac{1}{\lambda}\left(1 - e^{\lambda(t-t_0)}\right)\|y_1 - y_2\|$

$$\Rightarrow \quad \Phi' = \| y(s;y_1) - y(s;y_2) \|$$
$$\leq \lambda \Phi + \| y_1 - y_2 \|$$
$$\leq e^{\lambda(t-t_0)} \| y_1 - y_2 \|$$

Comments

Aside from proving the comforting fact that y depends continuously on y_0, it gives the discomfiting possibility of rapid, exponential divergence of orbits in time.

However, this is only an inequality, i.e., a bound.

Does warn against being able to compute reliably the long-time behavior of a system.

One-step methods

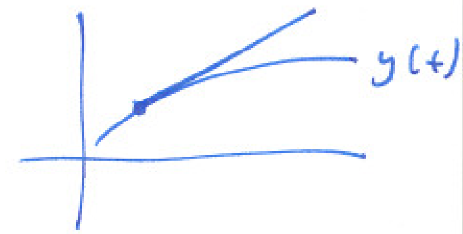
$$\frac{dy}{dt} = f(y,t) \quad , \quad y(t_0) = y_0$$

$$\Rightarrow \quad y(t) = y_0 + \int_{t_0}^{t} ds\, f(y(s), s)$$

Find a "local" solution to this equation.

$$y(t) \simeq y_0 + (t-t_0)\, f(y_0, t_0)$$

local affine approx. to $y(t)$



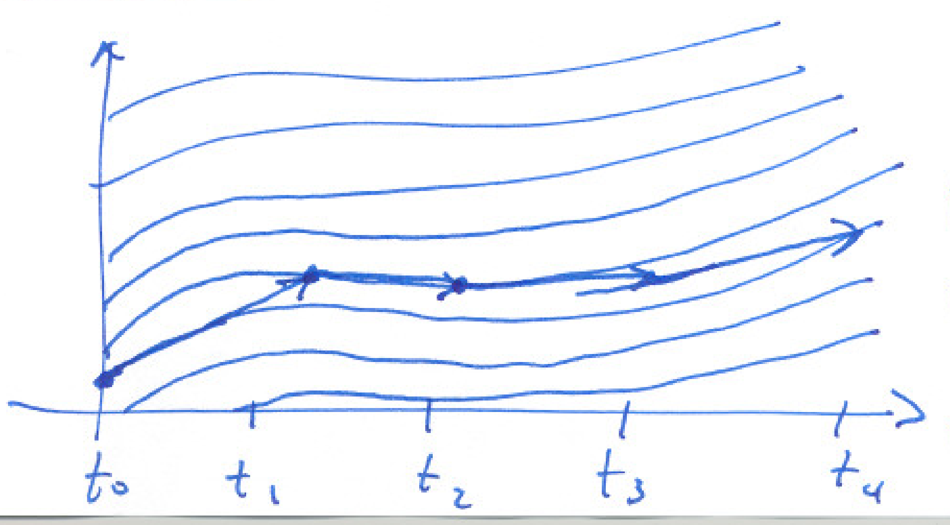
Set $t_1 = t_0 + h$

$$y(t_1) \simeq y_1 = y_0 + h\, f(y_0, t_0)$$

set $t_n = t_{n-1} + h$ to form the sequence

$$\boxed{y_n = y_{n-1} + h\, f(y_{n-1}, t_{n-1})}$$

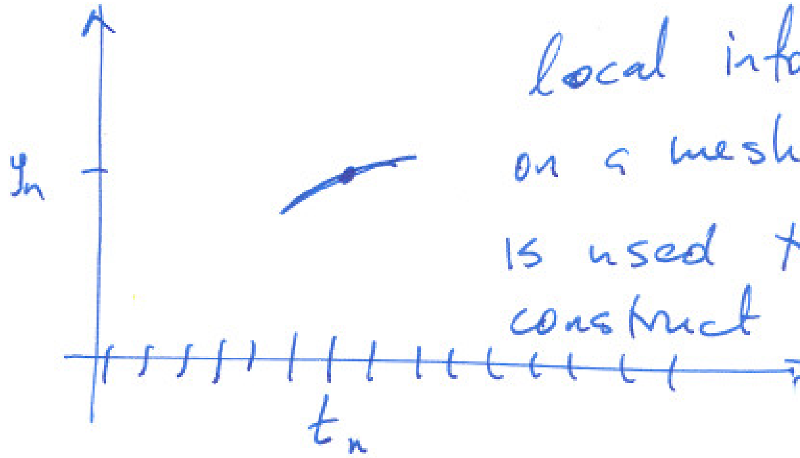
Called Euler's Method



Wandering from solution to solution.

E.M. is the starting point for understanding most methods for solving ~~ODEs~~ IVPs.

Main point:



local information on a mesh of pts. is used to construct local approx.

~~E.M. is the starting point for understanding most integration schemes.~~

How accurate is it?

<u>Simple case:</u> $f(y,t) = f(t)$

$$y(T) = y_0 + \int_0^T ds\, f(s)$$

set $h = T/N$, & let $h \to 0$.

$$y_N = y_0 + h\left[f_0 + f_1 + \dots + f_{N-1} \right]$$

$$= \underbrace{y_0 + h \sum_k{}'' f_k}_{\substack{2^{nd}\text{-order approximation} \\ \text{to } y(T)}} + \frac{h}{2}\left(f_0 - f_N\right)$$

$$\Rightarrow \left| y(T) - y_N \right| \leq A \cdot h$$

1^{st}-order method. ~~in this~~

Another example

$$\frac{dy}{dt} = \lambda y \,, \quad y(0) = y_0 > 0$$

Analytical $\quad y(t) = y_0 e^{\lambda t}$

Approx $\quad$ Fix $t = N \cdot h$

$$y_{n+1} = y_n + \lambda \cdot h \cdot y_n = (1+\lambda h) y_n$$

$$\Rightarrow \; y_N = (1+\lambda \cdot h)^N y_0$$

$$= (1+\lambda \cdot h)^{t/h} \, y_0$$

$$\Rightarrow \; \ln y_N = \frac{t}{h} \ln(1+\lambda h) + \ln y_0$$

$$\simeq \frac{t}{h}\left(\lambda h + \mathcal{O}(h^2)\right) + \ln y_0$$

$$\cancel{y_N = e^{[\lambda t + \mathcal{O}(h)]} y_0 \to e^{\lambda t} y_0 = y(t)}$$

Error $\quad y_N = y_0 \, e^{\lambda t + \mathcal{O}(h)} = y(t) + \mathcal{O}(h)$

Again, 1st order.

More rigorously.

Let $y_n = y_{n,h}$, $n = 0, 1, \dots, [t/h]$

E.M. is said to be convergent if, for every ODE w. Lipschitz cont. function f & for every $t > 0$, it is true that

$$\lim_{h \downarrow 0} \max_{n=0,1,\dots,[t/h]} \| y_{n,h} - y(t_n) \| = 0$$

Pf. Assume stronger condition that f is continuously differentiable, so that

$$|y(t+h) - (y(t) + h y'(t))| \leq C h^2 \text{ for } t \in [t_0, t]$$

Let $e_{n,h} = y_{n,h} - y(t_n)$

$$e_{0,h} = 0$$

$$
\begin{aligned}
e_{n+1,h} &= y_{n+1,h} - y(t_{n+1}) \\
&= y_{n,h} + \cancel{2}hf(y_{n,h}, t_n) \\
&\quad - \Big[y(t_n+h) - y(t_n) - hy'(t_n)\Big] \\
&\quad - \big(y(t_n) + hf(y(t_n), t_n)\big) \\
&= e_{n,h} + h\Big[f(y(t_n)+e_{n,h}, t_n) - f(y(t_n), t_n)\Big] \\
&\quad - \Big[y(t_n+h) - y(t_n) - hy'(t_n)\Big]
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \|e_{n+1,h}\| &\leq \|e_{n,h}\| + h\|f(y(t_n)+e_{n,h}, t_n) - f(y(t_n), t_n)\| \\
&\quad + Ch^2 \\
&\leq (1+\lambda h)\|e_{n,h}\| + Ch^2
\end{aligned}
$$

set $\xi_n = \| e_{n,h} \|$, $\xi_0 = 0$

$$\xi_{n+1} - (1+\lambda h)\,\xi_n \le c h^2$$

Let $\xi_n = (1+\lambda h)^n \mu_n$; Req: $\lambda h < 1$

$$\mu_{n+1} - \mu_n \le \frac{c h^2}{(1+\lambda h)} \left(\frac{1}{1+\lambda h} \right)^n$$

Sum over n

$$\Rightarrow \sum_{k=0}^{n-1} (\mu_{k+1} - \mu_k) = \mu_n$$

$$\le \frac{c h^2}{(1+\lambda h)} \sum_{k=0}^{n-1} \left(\frac{1}{1+\lambda h} \right)^k$$

$$= \frac{c h^2}{1+\lambda h} \, \frac{1 - \left(\frac{1}{1+\lambda h} \right)^n}{1 - \left(\frac{1}{1+\lambda h} \right)} = \boxed{\cancel{\frac{c}{\lambda} h \left[\left(\frac{1}{1+\lambda h} \right)^N - 1 \right]}}$$

$$\cancel{\Rightarrow \xi^N \le \frac{c}{\lambda} h \left[1 - (1-\lambda h)^N \right] = \frac{c}{\lambda} \cdot h \cdot \left[1 - (1-\lambda h)^{t/h} \right]}$$

$$\Rightarrow \xi_n^* \le \frac{c}{\lambda} \cdot h \cdot \left[(1+\lambda h)^n - 1 \right]$$

$$= \frac{c}{\lambda} \cdot h \cdot \left[(1+\lambda h)^{t_n/h} - 1 \right]$$

Use that $1 + \lambda \cdot h \le e^{\lambda h}$

$$\xi_n^* \le \frac{c}{\lambda} \cdot h \cdot \left[e^{\lambda \cdot t_n} - 1 \right] \le \frac{c}{\lambda} \cdot h \cdot \left[e^{\lambda t^*} - 1 \right]$$

~~independent of n.~~

~~$\xi^n \to 0$ as $h \downarrow 0$. i.e. convergent.~~

$$\| y_{n,h} - y(t_n) \| \le \frac{c}{\lambda} \left[e^{\lambda t^*} - 1 \right] \cdot h$$

uniformly in n.

Euler's Method is <u>first-order</u>. & convergent.

Implicit Euler (Also, 1^{st}-order & convergent)

$$y_{n+1} = y_n + h\, f(y_{n+1}, t_{n+1})$$

Trapezoidal [also implicit]

$$y_{n+1} = y_n + \frac{h}{2}\left[f(y_n, t_n) + f(y_{n+1}, t_{n+1}) \right]$$

Iserles: Trap. is convergent & 2^{nd}-order.

$$\| e_{n,h} \| \leq C h^2 .$$

Read Chap's 1 & 2.

H.W. 1.1, 1.4, 1.5, 1.7, 1.8

Euler's Method

$$y_{n+1} = y_n + h\, f(y_n, t_n) = y_n + \Phi_n$$

"Local ~~Trnc~~ Consistency Error"

$$= E[y] = y(t+h) - y(t) - h f(y(t), t)$$

$$= y(t) + h y'(t) + \tfrac{1}{2} h^2 y''(\xi) - y(t) - h f(y(t), t)$$

$$= \tfrac{1}{2} h^2 y''(\xi)$$

Local Consistency Error is 2nd order for Euler's Method. Global error is 1st order.

Trapezoidal Rule

$$y_{n+1} = y_n + \frac{h}{2}\left[f_{n+1} + f_n\right]$$

$$E[y] = y(t+h) - y(t) - \frac{h}{2}\left[f(y(t+h), t+h) + f(y(t), t)\right]$$

$$= y(t) + h y'(t) + \frac{h^2}{2} y''(t) - y(t) + O(h^3)$$

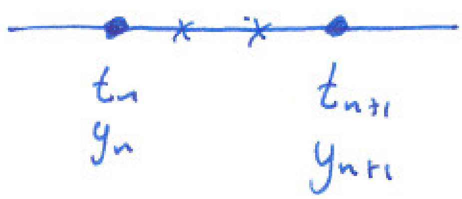
$$- \frac{h}{2}\left[\cancel{f(y,t)}\ f(y,t) + h y'(t) f_y + h f_t + O(h^2) + f(y,t)\right]$$

$$y''(t) = f_y f + f_t$$

$= O(h^3)$; LCE is 3rd-order.

Runge-Kutta Methods

- Generalization of E.M.
- single-step methods (self-starting)



y_{n+1} depends only upon y_n, though evaluation of y_{n+1} may depend upon evaluation of f within the interval $[t_n, t_{n+1}]$

Quadrature based method:

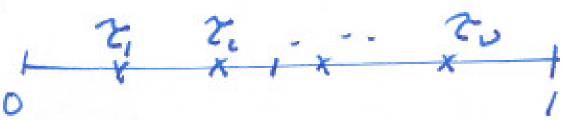
$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} ds\, f(y(s), s)$$

$$= y(t_n) + h \int_0^1 d\tau\, f(t_n + h\cdot\tau,\ y(t_n + h\cdot\tau))$$

Quadrature points τ_j with wghts b_j:

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j\, f(t_n + h c_j,\ y(t_n + h c_j))$$

However, $y(t_n + h c_j)$ is not known.



ordered.

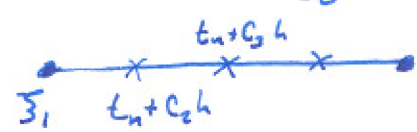
(Explicit) R-K Methods

Replace $y(t_n + h c_j)$ w. approximants ξ_j

$$y_{n+1} = y_n + h \sum_{j=1}^{\nu} b_j f(t_n + h c_j, \xi_j)$$

where ξ_j is determined recursively to depend

<u>only</u> upon $\xi_1, \dots, \xi_{j-1}$: Pick quad. scheme s.t. $\tau_0 = 0$ &



$$\begin{cases} \xi_1 = y_n \\ \xi_2 = y_n + h\, a_{2,1} f(\xi_1, t_n) \\ \xi_3 = y_n + h\, a_{3,1} f(\xi_1, t_n) + h a_{3,2} f(\xi_2, t_n + c_2 h) \\ \vdots \\ \xi_\nu = y_n + \sum_{i=1}^{\nu-1} a_{\nu,i} f(\xi_i, t_n + c_i \cdot h) \end{cases}$$

$$\underline{\underline{A}} = \left(\begin{array}{ccc|c} 0 & 0 & 0 & 0 \\ \hline a_{2,1} & 0 & 0 & 0 \\ a_{3,1} & a_{3,2} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ a_{\nu,1} & a_{\nu,2} & a_{\nu,\nu-1} & 0 \end{array} \right)$$

RK matrix, lower triangular.

How to choose $\underline{A}$ (and $\underline{b}$ & $\underline{c}$)?

Maximize the order of the LCE. $E[y]$.

$\underline{\nu = 2}$ $\quad A = \begin{pmatrix} 0 & 0 \\ a_{21} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ a & 0 \end{pmatrix}$, $\quad c_2 = c$

4 unknowns.

$$\xi_1 = y_n$$

$$\xi_2 = y_n + a \cdot h f(\xi_1, t_n)$$

$$y_{n+1} = y_n + h\left[b_1 f(\xi_1, t_n) + b_2 f(\xi_2, t_n + c_2 h)\right]$$

$$E[y] = y(t+h) - y(t) - h\left[b_1 f(y,t) + b_2 f(y + a \cdot h f(y,t), t + ch)\right]$$

$$= h y'(t) + \tfrac{1}{2} h^2 y''(t) + \tfrac{1}{2} h^3 y'''(t) + \cdots - h b_1 f(y,t)$$

$$- b_2 h \underbrace{f(y + a \cdot h \cdot f(y,t), t + ch)}$$

$$= f(y,t) + a \cdot h f f_y + c \cdot h f_t + h^2 P$$

$$= h\left[y' - (b_1 + b_2) f\right] + h^2\left[\tfrac{1}{2} y'' - a b_2 f f_y - c b_2 f_t\right]$$

$$+ h^3\left[y'''(t) - P\right] + \mathcal{O}(h^4).$$

choose a, b_1, b_2, & c to eliminate as many orders as possible – (Method of undetermined coefficients.)

$\underline{O(h)}$: $\boxed{1 = b_1 + b_2}$

$O(h^2)$: $y' = f(y,t) \Rightarrow y'' = f_y f + f_t$

$$\Rightarrow \boxed{\frac{1}{2} = a b_2 \,, \quad \frac{1}{2} = c b_2} \Rightarrow a = c$$

3 relations, 4 unknowns $\Rightarrow$ under-determined
1 dim'l manifold of methods.

$\underline{O(h^3)}$ $\quad y''' = f_{yy} f^2 + 2 f_{yt} f + f_y f_t + f_{tt}$

Eliminating this order will generate at least 4 add'l conditions. The system will then be over-determined. (& generally have no solution)

Thus, this can generate a 3rd order LCE at best. ($\Rightarrow$ 2nd-order global error).

Thus, there are an infinite # of 2nd-order Explicit R-K schemes.

Examples

(1) $b_1 = 0 \Rightarrow b_2 = 1, \quad a = \frac{1}{2}, \quad c = \frac{1}{2}$

$$\begin{cases} \xi_1 = y_n \\ \xi_2 = y_n + \frac{1}{2} h f(y_n, t_n) \\ y_{n+1} = y_n + h f(\xi_2, t_n + \frac{1}{2}h) \\ \quad \left[= y_n + h f\left(y_n + \frac{1}{2} h f(y_n, t_n), t_n + \frac{1}{2} h\right)\right] \end{cases}$$

$f(y, t) = f(t)$

$$\Rightarrow y_{n+1} = y_n + h f(t_n + \tfrac{1}{2} h)$$

$$= y_0 + h \sum_{k=0}^{n} f((j + \tfrac{1}{2})h)$$

The midpoint rule.

(2) $c = 1$ (evaluation at the end-point)

$\Rightarrow b_2 = \frac{1}{2} = b_1$; $a = 1$.

$$\begin{cases} \xi_1 = y_n \\ \xi_2 = y_n + h f(\xi_1, t_n) \\ y_{n+1} = y_n + \frac{h}{2}\left[f(\xi_1, t_n) + f(\xi_2, t_n + h) \right] \end{cases}$$

Another variant of the trapezoidal rule.
(usually called RK2)

RK4

Most popular.

$k_1 = f(\xi_1)$

$$\begin{cases} \xi_1 = y_n \\ \xi_2 = y_n + \frac{h}{2} \cancel{f(\xi_1, t_n)} = y_n + \frac{h}{2} k_1, \quad k_2 = f(\xi_2) \\ \xi_3 = y_n + \frac{h}{2} f(\xi_2, t_n + \frac{1}{2}h) = y_n + \frac{h}{2} k_2 \\ \xi_4 = y_n + h f(\xi_3, t_n + h) = y_n + h k_3 \end{cases}$$

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$= y_n + \frac{h}{6}\left[f(\xi_1, t_n) + 2 f(\xi_2, t_n + \tfrac{1}{2}h) + 2 f(\xi_3, t_n + \tfrac{1}{2}h) + f(\xi_4, t_n + h) \right]$$

RK4 - Most popular

$$k_1 = \cancel{h} f(y_n, t_n)$$

$$k_2 = \cancel{h} f(y_n + \tfrac{1}{2}hk_1, t_n + \tfrac{h}{2})$$

$$k_3 = \cancel{h} f(y_n + \tfrac{1}{2}hk_2, t_n + \tfrac{h}{2})$$

$$k_4 = \cancel{h} f(y_n + hk_3, t_n + h)$$

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$\xi_1 = y_n \qquad k_1 = f(\xi_1, t_n)$$

$$\xi_2 = y_n + \frac{h}{2}k_1, \quad k_2 = f(\xi_2, t_n + \tfrac{h}{2})$$

$$\xi_3 = y_n + \frac{h}{2}k_2, \quad k_3 = f(\xi_3, t_n + \tfrac{h}{2})$$

$$\xi_4 = y_n + k_3, \quad k_4 = f(\xi_4, t_n + h)$$

$E[y] = O(h^5)$; 4^{th} order method.

$f(y,t) = f(t)$

$$y_{n+1} - y_n = \frac{h}{6}\left[f(t_n) + 4f(t_n + \tfrac{1}{2}h) + f(t_n + h)\right]$$

Simpson's Rule!

Convergence of Single-step methods in outline
(really identical to that for Euler)

<u>S.S. Method</u>: $y_{n+1} = y_n + h\,\Phi[y_n, t_n; h]$

~~Ex:~~ RK2:

$$\Phi[y,t;h] = \frac{1}{2}\left[f(y,t) + f(y + hf(y,t), t+h)\right]$$

<u>Local Consistency Error:</u>

$$E[y,t;h] = y(t+h) - y(t) - h\,\Phi[y,t;h]$$

<u>RK2:</u> $E[y,t;h] \le Ch^3$

p^{th}-order method: $|E[y,t;h]| \le Ch^{p+1}$

<u>"Lifschitz" Condition (assumed)</u>: $\exists\, h_0$ s.t. $\forall\, h \le h_0$

$$\|\Phi[y_*, t; h] - \Phi[z_*, t; h]\| \le M\|y_* - z_*\|$$

Follows from L. Condition on f.

RK2:

$$\|\Phi[y,t;h] - \Phi[z,t;h]\|$$

$$\le \frac{1}{2}\Big\|\big(f(y,t) - f(z,t)\big) + \big(f(y+hf(y,t),t+h) - f(z+hf(z,t),t+h)\big)\Big\|$$

$$\le \frac{1}{2}\Big\{\lambda\|y-z\| + \lambda\big\|\cancel{f}(y-z) + h\big(f(y,t) - f(z,t)\big)\big\|\Big\}$$

$$\le \frac{1}{2}\Big\{2\lambda\|y-z\| + \lambda^2 h\|y-z\|\Big\}$$

$$= \left(1 + \frac{1}{2}\lambda h\right)\lambda\|y-z\| \le 2\lambda\|y-z\|$$ for

$$\lambda h \le \lambda h_0 = 2$$

Lemma: If $|\xi_{n+1}| \le (1+\delta)|\xi_n| + B$, $\delta, B > 0$

then $|\xi_n| \le e^{n\delta}|\xi_0| + \dfrac{e^{n\delta}-1}{\delta}B$

Pf: (telescoping sum)

$$\sum_{k=0}^{n}\left\{\frac{|\xi_{k+1}|}{(1+\delta)^{k+1}} - \frac{|\xi_k|}{(1+\delta)^k} \le \frac{B}{(1+\delta)^{k+1}}\right\} \Rightarrow \frac{|\xi_{n+1}|}{(1+\delta)^{n+1}} - |\xi_0| \le \frac{B}{1+\delta}\,\frac{1-(1+\delta)^{-(n+1)}}{1-(1+\delta)^{-1}}$$

$$\Rightarrow |\xi_{n+1}| \le (1+\delta)^{n+1}|\xi_0| + \frac{B}{\delta}\left[(1+\delta)^{n+1} - 1\right]$$

& use $1+\delta \le e^{\delta}$ for $\delta \ge 0$

$$\Rightarrow |\xi_n| \le e^{n\delta}|\xi_0| + \frac{B}{\delta}(e^{n\delta}-1)$$

Convergence proof:

Given a $p^{\underline{th}}$-order method ~~satis~~ w. Φ satisfying the Lipschitz condition:

$$e_{n+1} = y_{n+1} - y(t_{n+1})$$

$$= y_n + h\,\Phi[y_n, t_n; h] - E[y, t_n; h]$$

$$-y(t_n) - h\,\Phi[y(t_n), t_n; h]$$

$$= e_n + h\Big[\Phi[y(t_n)+e_n, t_n; h] - \Phi[y(t_n), t_n; h]\Big]$$

$$-E[y, t_n; h]$$

$$\Rightarrow \|e_{n+1}\| \le (1+hM)\|e_n\| + Ch^{p+1}$$

Apply the lemma, w. $|\xi_0| = \|e_0\| = 0$, $\delta = hM$, $B = Ch^{p+1}$

$$\|e_n\| \le \frac{Ch^{p+1}}{hM}(e^{n\cdot h\cdot M}-1)$$

$$\le \frac{C}{M}(e^{Mt_n}-1)h^p \le \frac{C}{M}(e^{Mt^*}-1)h^p$$

for $t_n \le t^* < \infty$

Let $\tilde{y}(t;h) = y_M$ where $h = (t-t_0)/M$.

<u>Thm</u> (Stoer & Bulirsch p. 443) Let $f \in C^{N+2}[S]$ & let $\tilde{y}(t;h)$ be the approximate solution obtained by a p^{th}-order, one-step method, $p \leq N$, to the IVP

$$\frac{dy}{dt} = f(y,t), \quad y(t_0) = y_0, \quad x_0 \in [a,b].$$

Then $\tilde{y}(t;h)$ has an asymptotic expansion of the form

$$\tilde{y}(t;h) = y(t) + e_p(t)h^p + e_{p+1}(t)h^{p+1} + \cdots$$
$$+ h^N e_N(t) + h^{N+1}\tilde{E}_{N+1}(t;h)$$

with $e_k(t_0) = 0 \quad k = p, p+1, \ldots$

valid for all $t \in [a,b]$ and all $h = (t-t_0)/n$, $n = 1, 2, \ldots$ The remainder term $\tilde{E}_{N+1}(t;h)$ is bdd for fixed t & all $h_n = (t-t_0)/n$.

Let $\tilde{y}(t;h) = y_M$ where $h = t/M$. Then, we have the following useful fact:

<u>Thm</u> (Stoer & Bulirsch) Let $f \in C^N$

Sketch of proof (constructive side)

For a ~~step~~ method of order p, can write

$$E[y(t),t;h] = y(t+h) - y(t) - h\,\Phi[y(t),t;h]$$

$$= d_{p+1}(t)\,h^{p+1} + d_{p+2}(t)\,h^{p+2} + \cdots$$

Use this expansion to construct $e_p, e_{p+1}, \ldots$

Assuming $e_p(t)$ exists, ~~consider~~ then

$$\tilde{y}(t;h) - y(t) = e_p(t)\,h^p + O(h^{p+1})$$

Consider the new approximation

$$\hat{y}(t;h) = \tilde{y}(t;h) - e_p(t)\,h^p$$

Then $\hat{y}$ is constructed from the 1-step method:

$$\hat{\Phi}(y,t;h) = \Phi(y + e_p(t)\,h^p, t; h)$$

$$- (e_p(t+h) - e_p(t))\,h^{p-1}$$

Check: $\hat{y}_{n+1} = \hat{y}_n + h\Big\{\Phi(\hat{y}_n + e_p(t_n)\,h^p, t_n; h)$

$$- (e_p(t_n+h) - e_p(t_n))\cdot h^{p-1}\Big\}$$

$$\Leftrightarrow \left(\hat{y}_{n+1} + e_p(t_n+h)h^p\right) = \left(\hat{y}_n + e_p(t_n)h^p\right) + h\Phi\left[\hat{y}_n + e_p(t_n)h^p, t_n; h\right]$$

$$\Leftrightarrow \tilde{y}_{n+1} = \underline{\tilde{y}_n + h\Phi}(y_n, t_n; h) \checkmark$$

Then, $\hat{E}[y,t;h] = y(t+h) - y(t) - h\hat{\Phi}[y,t;h]$

$$= y(t+h) - y(t) - h\Phi[y,t;h] + h\left[\Phi[y,t;h] - \hat{\Phi}[y,t;h]\right]$$

$$= d_{p+1}(t)h^{p+1} + O(h^{p+2}) + h\left\{\Phi[y,t;h] - \Phi[y + e_p(t)h^p, t; h] - \frac{(e_p(t+h) - e_p(t))}{h}h^p\right\}$$

$\Big\downarrow$ Expand in h

$$= d_{p+1}(t)h^{p+1} + O(h^{p+2}) - h\,e_p(t)h^p \frac{\partial\Phi}{\partial y}[y,t;0] - e_p'(t)h^{p+1} + O(h^{p+2})$$

~~Assume lim~~ $\lim_{h\downarrow 0} \Phi[y,t;h] = f(y,t)$

$$\frac{\partial f}{\partial y} = \lim_{h\downarrow 0} \frac{\partial \Phi}{\partial y}[y,t;h]$$

Check $\hat{y}_{n+1} = \hat{y}_n + h\left[\Phi(\hat{y}_n + e_p(t_n)h^p, t_n; h) - \frac{e_p(t_n+h) - e_p(t_n)}{h} h^{p}\right]$

or

$$= h^{p+1}\left[d_{p+1}(t) - \left(e_p' + e_p(t)\,\frac{\partial f}{\partial y}(y,t)\right)\right] + O(h^{p+2})$$

$\Rightarrow$ Take $e_p(t)$ to satisfy

$$\boxed{\frac{de_p}{dt} = d_{p+1}(t) - \frac{\partial f}{\partial y}(y(t),t)\,e_p(t)} \qquad e_p(0) = 0.$$

Why is this useful

1.) Can build new methods – see S&B.

2.) Can be utilized for time-step control

3.) Very useful for debugging code

Ratio Test:

~~$\text{error} = e_p(t)\,h^p$~~

$$e(t;h) = \tilde{y}(t;h) - y(t) = e_p(t)\,h^p + O(h^{p+1})$$

$$\Rightarrow R = \frac{\tilde{y}(t;h) - \tilde{y}(t;\frac{h}{2})}{\tilde{y}(t;\frac{h}{2}) - \tilde{y}(t;\frac{h}{4})} \approx \frac{h^p - (\frac{h}{2})^p}{(\frac{h}{2})^p - (\frac{h}{4})^p}$$

$$= \frac{1}{(1/2)^p} = 2^p!$$

$\frac{RK4}{RK2}$ $\quad R = 16$

$\quad\quad\quad R = 4$

Other Topics

- Implicit R-K methods.

  Here, the matrix $\underline{\underline{A}}$ is <u>not</u> lower triangular, but, instead, is full.

  <u>Text</u> "Two-stage" IRK method

$$
(1)\begin{cases}
\xi_1 = y_n + \frac{1}{4}h\left[f(\xi_1, t_n) - f(\xi_2, t_2 + \frac{2}{3}h)\right] \\
\xi_2 = y_n + \frac{1}{12}h\left[3f(\xi_1, t_n) + 5f(\xi_2, t_n + \frac{2}{3}h)\right]
\end{cases}
$$

$$
(1') \quad y_{n+1} = y_n + \frac{1}{4}h\left[f(\xi_1, t_n) + 3f(\xi_2, t_n + \frac{2}{3}h)\right]
$$

This is a third-order scheme (LCE is 4^{th} order)

- Req's solution of Eqs (1) at each step, which is a set of nonlinear eqns.
- More unknowns allows an increase in order.

There is also a two-stage, <u>fourth-order method</u> using Gaussian quadrature. | $c_1 \neq 0$, determine all the nodal points.

Two areas where issues of how time-stepping is done are

1.) Comp'l PDE

Fluid Mechanics

Optics ...

2.) Molecular Dynamics

Both typified by having many, many degrees of freedom, (i.e. many eqns) and many time-scales.

After Discretization

$$\frac{d\underline{X}}{dt} = \underline{F}(\underline{X}(t), t)$$

General Issues

0.) Cost of evaluation of F.

1.) Accuracy - do you need it?

2.) Stability - keep "small-scales" under control.

3.) Time-step control

Simple problem

$$u_t = \nu u_{xx} \qquad u \in C_p^\infty[0, 2\pi]$$

$$u = \sum_{k=-N/2}^{N/2} \hat{u}_k(t) e^{ikx}$$

$\Delta x = 2\pi/N$

$$\frac{d\hat{u}_k}{dt} = -\nu |k|^2 \hat{u}_k \qquad \mathring{a} = -\lambda a$$

$$a = e^{-\lambda t} a_0$$

Euler

$$a_{n+1} = (1 - \lambda \cdot \Delta t) a_n = (1 - \lambda \Delta t)^n a_0$$

Req. $a_n \to 0$ as $n \to \infty$

$$\underbrace{-1 \le 1 - \lambda \Delta t} \le 1$$

$$\lambda \Delta t \le 2$$

$$\Delta t \le 2/\lambda = \frac{2}{\nu |k|^2} \le \frac{2}{\nu} \frac{1}{N^2/4} = \frac{8}{\nu} \frac{\Delta x^2}{(2\pi)^2}$$

$$\boxed{\Delta t \le \frac{A}{\nu} \Delta x^2}$$ // A-stability region

Implicit E.

$$a_{n+1} = a_n - \lambda \Delta t \, a_{n+1}$$

$$\Rightarrow a_{n+1} = \frac{1}{1+\lambda \Delta t} a_n = \left(\frac{1}{1+\lambda\Delta t}\right)^n a_n$$ // always stable.

Trapezoidal Rule or Crank-Nicholson

$$\frac{a_{n+1} - a_n}{\Delta t} = -\frac{1}{2}\lambda (a_{n+1} + a_n)$$

2nd-order!

$$\left(1 + \tfrac{1}{2}\lambda\Delta t\right) a_{n+1} = \left(1 - \tfrac{1}{2}\lambda\Delta t\right) a_n$$

$$a_{n+1} = \frac{1 - \frac{1}{2}\lambda\Delta t}{1 + \frac{1}{2}\lambda\Delta t} a_n = \frac{1-\alpha}{1+\alpha} a_n$$

$$-1 < \frac{1-\alpha}{1+\alpha} < 1$$

$$-1 \cancel{-\alpha} < \cancel{1-\alpha} < 1+\alpha$$

Read 1, 2, 3, 4, 5

Generally, consider problems of the form

$$u_t = \mathcal{L}[u]$$, where $\mathcal{L}$ is

diagonalized by the Fourier tf.

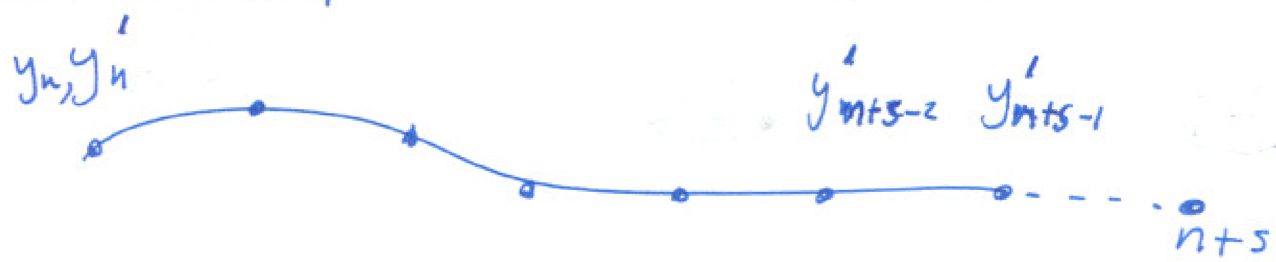
$$\hat{u}_t = -g_k \hat{u}$$

Multi-step Methods

$$\frac{dy}{dt} = f(y,t) \ , \quad t \geq t_0 \ , \quad y(t_0) = y_0$$

Idea: Use past values of y & y'

The point: Economy.



Begin w. $$y(t_{n+s}) = y(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} d\tau \ y'(\tau)$$

Adams Method Use past values of the solution to approx. $y'(t)$.

Let the polynomial $p(t)$ interpolating $f(y_k, t_k)$ for $k = n, \ldots, n+s-1$

$$p(t) = \sum_{m=0}^{s-1} p_m(t) \, f(y_{n+m}, t_{n+m})$$

$p_m(t)$ are Lagrange polynomials

$$p_m(t) = \prod_{\substack{l=0 \\ l \neq m}}^{s-1} \frac{t - t_{n+l}}{t_{n+m} - t_{n+l}} \qquad p_m(t_{n+m}) = 1$$
$$p_m(t_{n+l}) = 0 \quad l \neq m$$

Then ~~1.) $p(t_m) = f(y_m, t_m), \ldots$~~

1.) $p(t_k) = f(y_k, t_k)$, $k = n, n+1, \ldots, n+s-1$

2.) $p(t) = y'(t) + O(h^s)$

~~on~~ for $t \in [t_{n+s-1}, t_{n+s}]$

i.e., local extrapolation error. of polynomial interpolation.

~~$y_{n+s} = y_{n+s-1} + h \sum_{m=0}$~~

Suggests approximation:

$$y_{n+s} = y_{n+s-1} + \int_{t_{n+s-1}}^{t_{n+s}} d\tau \sum_{m=0}^{s-1} p_m(\tau)\, f(y_{n+m}, t_{n+m})$$

$$= y_{n+s-1} + \underbrace{\sum_{m=0}^{s-1} \left[\int_{t_{n+s-1}}^{t_{n+1}} d\tau\, p_m(\tau) \right]}_{\text{independent of } n.} f(y_{n+m}, t_{n+m})$$

$$\int_{t_{n+s-1}}^{t_{n+s}} d\tau\, p_m(\tau) = \int_{t_{n+s-1}}^{t_{n+s}} d\tau \left[\prod_{\substack{l=0 \\ l \neq m}}^{s-1} \frac{\tau - t_{n+l}}{t_{n+m} - t_{n+l}} \right]$$

$$u = s - t_0 = (v+n)h$$

$$s = t_0 + (v+n)h$$

$$= \int_{t_0+(n+s-1)h}^{t_0+(n+s)h} d\tau \left[\prod_{\substack{l=0 \\ l \neq m}}^{s-1} \frac{\tau - t_0 - (n+l)h}{\underbrace{(n+m)h - (n+l)h}_{(m-l)h}} \right]$$

set $v = (\tau - t_0 - nh)/h$

$$= h \int_{s-1}^{s} dv \prod_{l=0}^{s-1} \frac{v-l}{m-l}$$

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s-1} b_m f(y_{n+m}, t_{n+m})$$

Local Consistency Error

$$E[y,t;h] = y(t_s) - y(t_{s-1}) - h \sum_{m=0}^{s-1} f(y(t_m), t_m)$$

$$= \mathcal{O}(h^{s+1})$$

Called Adams-Bashforth methods.

$\underline{s=1}$ $\quad y_{n+1} = y_n + hf(y_n, t_n)$

$\underline{s=2}$ $\quad y_{n+2} = y_{n+1} + h\underbrace{\left[\frac{3}{2}f(y_{n+1}, t_{n+1}) - \frac{1}{2}f(y_n, t_n)\right]}_{\text{polynomial extrapolation.}}$

$\underline{s=3}$ $\quad y_{n+3} = y_{n+2}$

$$+ h\left[\frac{23}{12}f_{n+2} - \frac{4}{3}f_{n+1} + \frac{5}{12}f_n\right]$$

Each of the methods requires only one fcn evaluation per time-step. Economical.

- As these are not single-step methods, they require a "start-up" method.

$\underline{s=2)}$ $\quad f_0 \quad f_1 \to y_2$

$\uparrow$

need to approximate ~~this~~ y_1.

Use Euler to achieve global error of h^2?

i.e. start-up can be one less order.

<u>More generally</u> we might write

$$y_{n+s} + \sum_{m=0}^{s-1} \alpha_m y_{n+m} = h \sum_{m=0}^{s} b_m f(t_{n+m}, y_{n+m}) \qquad (\star)$$

$\alpha_s = 0$ (normalization)

$b_s = 0 \Rightarrow$ explicit, otherwise implicit.

(A (linear) multi-step method)

The method is of order s if

$$E[y, t, h] = y(t_{n+s}) + \sum_{m=0}^{s-1} \alpha_m y(t_{n+m})$$

$$- h \sum_{m=0}^{s} b_m f(y(t_{n+m}), t_{n+m})$$

$$= O(h^{s+1})$$

[$s \geq 1$ is called a consistent method]

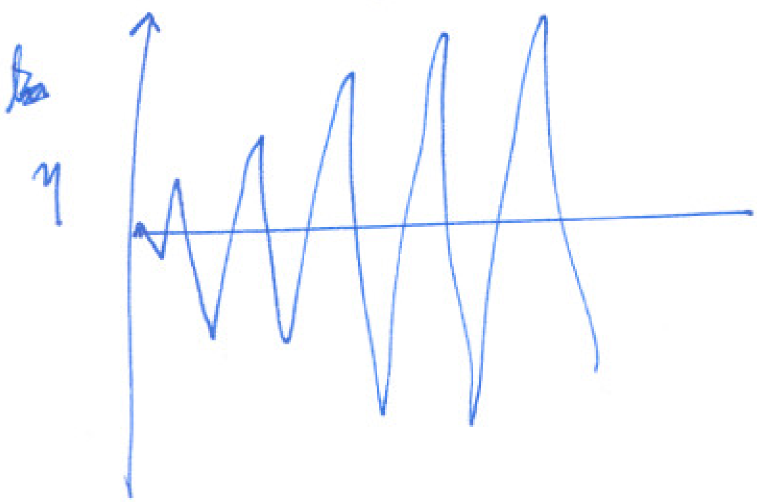
Does consistency equal convergence, as for one-step methods?

A 3rd-order multi-step method:

$$y_{i+2} + 4y_{i+1} - 5y_i = h[4f(y_{i+1}, t_{i+1}) + 2f(y_i, t_i)]$$

Consider $\frac{dy}{dt} = -y$, $y(0) = 1 \Rightarrow y(t) = e^{-t}$

Begin w $y_0 = 1$, $y_1 = e^{-h}$, i.e. exact soln.



w. exponential growth,

---

what is going on? Consider the discrete eqn

$$y_{i+2} + 4y_{i+1} - 5y_i = h[-4y_{i+1} - 2y_i]$$

$$\Rightarrow \boxed{y_{i+2} + 4(1+h)y_{i+1} + (-5+2h)y_i = 0} \quad (*)$$

A linear difference equation

- Look for solutions $\eta_j = \xi^j$

$$\Rightarrow \xi^2 + 4(1+h)\xi + (-5+2h) = 0$$

two roots

$$\Rightarrow \begin{cases} \xi_1 = -2 - 2h + 3\left(1 + \frac{2}{3}h + \frac{4}{9}h^2\right)^{1/2} \\ \xi_2 = -2 - 2h - 3\left(1 + \frac{2}{3}h + \frac{4}{9}h^2\right)^{1/2} \end{cases}$$

Expand the roots in small h.

- $$\xi_1 = 1 - h + \frac{1}{2}h^2 - \frac{1}{6}h^3 + \frac{1}{72}h^4 + \mathcal{O}(h^5)$$

$$\xi_2 = -5 - 3h + \mathcal{O}(h^2) \qquad \text{Hmm...}$$

Solutions to Eq. (*) can be written generally as

$$\eta_j = \alpha \xi_1^j + \beta \xi_2^j$$

w. $\cancel{\eta_0 = \alpha \xi_1 + \beta \xi_2 = 1}$

$$\alpha + \beta = 1 = \eta_0$$
$$\alpha \xi_1 + \beta \xi_2 = e^{-h} = \eta_1$$

- $$\Rightarrow \alpha = \frac{\xi_2 - e^{-h}}{\xi_2 - \xi_1} \quad ; \quad \beta = \frac{e^{-h} - \xi_1}{\xi_2 - \xi_1} \neq 0.$$

with $\begin{cases} \alpha = 1 + O(h^2) \\ \beta = -\frac{1}{216} h^4 + O(h^5) \end{cases}$

Now, fix $t > 0$, $h = t/n$, look as $n \to \infty$.

$$\eta[t; h] = \alpha \xi_1^n + \beta \xi_2^n$$

$$= \left[1 + O\left(\left(\tfrac{t}{n}\right)^2\right)\right] \cdot \left[1 - \tfrac{t}{n} + O\left(\left(\tfrac{t}{n}\right)^2\right)\right]^n$$

$$- \frac{1}{216} \left(\frac{t}{n}\right)^4 \left[1 + O\left(\frac{t}{n}\right)\right]\left[-5 - 3\frac{t}{n} + O\left(\frac{t}{n}\right)^2\right]^n$$

$n \uparrow \infty$ $$\approx e^{-t} - \underbrace{\frac{t^4}{216} \frac{(-5)^n}{n^4} e^{3t/5}}_{\text{exponential divergence! as } n \to \infty}$$

~~Consider even $f = 0$~~

This arises from the fact that the ~~polynomial~~ poly eqn

$\mu^2 + 4\mu - 5 = 0$ has a

root of (-5).

So what? ~~[illegible]~~ Couldn't the initial condition be adjusted to remove this "branch" of solutions?

$$\alpha + \beta = \cancel{1}\eta_0 = 1$$

$$\alpha \xi_1 + \beta \xi_2 = \eta_1 \quad \text{~~choose an $\beta = 0$~~}$$

Choose $\beta = 0 \Rightarrow \alpha = 1, \; \eta_1 = \xi_1 \simeq e^{-h} + O(h^4)$

Nonetheless, round-off errors will inevitably introduce the 2^{nd} ξ_2 branch & errors will grow.

This is an example of a <u>consistent</u>, but <u>unstable</u> method.

Checking consistency

Consider the two polynomials

$$\rho(\omega) = \sum_{m=0}^{s} a_m \, \omega^m \qquad (\alpha_0 = 1)$$

$$\sigma(\omega) = \sum_{m=0}^{s} b_m \, \omega^m$$

Theorem The multi-step method $(\star)$ is of order $\tilde{s} \geq 1$ iff $\exists\, c \neq 0$ s.t.

$$\rho(\omega) - \ln\omega \cdot \sigma(\omega) = c(\omega-1)^{\tilde{s}+1} + \mathcal{O}(|\omega-1|^{\tilde{s}+2})$$

as $\omega \to 1$.

Pf. Assume $y(t)$ is analytic with radius of convergence greater that $s \cdot h$ (this places an a priori bound on h).

Expand $E[y, t; h]$ in small h.

$$\Rightarrow E[y,t;h] = \sum_{m=0}^{s} a_m y(t+mh)$$

$$- h \sum_{m=0}^{s} b_m y'(t+mh)$$

$$= \left(\sum_{m=0}^{s} a_m \right) y(t)$$

$$+ \sum_{k=1}^{\infty} \frac{1}{k!} \left[\sum_{m=0}^{s} a_m m^k - k \sum_{m=0}^{s} b_m m^{k-1} \right] h^k y^{(k)}(t)$$

Nec. & sufficient condition for method to be of order $\tilde{s}$

$$\sum_{m=0}^{s} a_m = 0 \;; \quad \sum_{m=0}^{s} m^k a_m = k \sum_{m=0}^{s} m^{k-1} b_m$$

$$k = 1, 2, \ldots, \tilde{s}$$

$$\sum_{m=0}^{s} m^{\tilde{s}+1} a_m \neq (\tilde{s}+1) \sum_{m=0}^{s} m^{\tilde{s}} b_m$$

(not of higher order)

Now, let $\omega = e^z$ & expand in $z \approx 0$.

$$\rho(\omega) - \sigma(\omega) \ln \omega = \rho(e^z) - z\,\sigma(e^z)$$

$$= \sum_{m=0}^{s} a_m \underset{\text{expand}}{e^{mz}} - z \sum_{m=0}^{s} b_m \underset{\text{expand}}{e^{mz}}$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{m=0}^{s} m^k a_m \right) z^k$$

$$- \sum_{k=1}^{\infty} \frac{1}{k!} \left(k \sum_{m=0}^{s} m^{k-1} b_m \right) z^k$$

$$= c\, z^{\tilde{s}+1} + O(z^{\tilde{s}+2})$$

$$|z| = |\ln \omega| = |\ln[1-(1-\omega)]| = |\omega - 1|$$

Examples

1.) Divergent multi-step method:

$$\rho(\omega) = -5 + 4\omega + \omega^2, \quad \sigma(\omega) = 2 + 4\omega$$

Let $\omega = 1 + \xi$ & expand in $|\xi| << 1$.

$$\rho(\omega) - \ln\omega \cdot \sigma(\omega)$$

$$= \left[-5 + 4(1+\xi) + (1+\xi)^2\right]$$

$$- \ln(1+\xi) \cdot \left[2 + 4\cancel{\omega}(1+\xi)\right]$$

$$\ln(1+\xi), \quad \frac{1}{1+\xi}, \quad \frac{-1}{(1+\xi)^2}, \quad \frac{2}{(1+\xi)^3}, \quad \ldots \frac{(-1)^{k+1}(k-1)!}{(1+\xi)^k}$$

$$= (6\xi + \xi^2) - (6 + 4\xi)\left[\xi - \frac{1}{2}\xi^2 + \frac{1}{3}\xi^3 - \frac{1}{4}\xi^4 + \ldots\right]$$

$$= (6\xi + \xi^2) - \left(6\xi - 3\xi^2 + 2\xi^3 + O(\xi^4)\right)$$

$$- \left(4\xi^2 - 2\xi^3 + O(\xi^4)\right)$$

$$= O(\xi^4) + \text{HOTs}.$$

2.) <u>AB2</u> $\quad \rho(\omega) - \ln\omega\, \sigma(\omega) = \frac{5}{12}\xi^3 + O(\xi^4)$

<u>Root Condition</u> A polynomial $\psi(\mu)$ obeys the root (or stability) condition if every zero ξ of ψ satisfies $|\xi| \le 1$, & if

$[\psi(\xi) = 0$ & $|\xi| = 1$ (on the disk)$]$ then

ξ is a <u>simple</u> zero.

(Dahlquist)
<u>Equivalence Thm</u> Suppose Error$[y_1, \dots, y_{s-1}] \downarrow 0$ as $h \downarrow 0^+$, Then the linear multi-step method is convergent <u>iff</u> it is of order $\tilde{s} \ge 1$, and ρ obeys the stability condition.

(Consistency + Stability $\Longleftrightarrow$ Convergence)

<u>Example 1</u>. Method fails the stability condition.

<u>AB2</u> $\rho(\omega) = \omega - 1$. A convergent method.

BDF Methods (Backward Differentiation Formulae)

Special case of multi-step formula, built for having good stability properties.

Recall $$\sum_{m=0}^{s} \alpha_m y_{n+m} = h \sum_{m=0}^{s} b_m f(y_{n+m}, t_{n+m})$$

Consider $$\sum_{m=0}^{s} \alpha_m y_{n+m} = h \beta f(y_{n+s}, t_{n+s})$$

i.e. $\sigma(\omega) = \beta \omega^s$, called a BDF.

Taking $\beta = 1 / \left(\sum_{m=1}^{s} \frac{1}{m} \right)$

$$\rho(\omega) = \beta \sum_{m=1}^{s} \frac{1}{m} \omega^{s-m} (\omega - 1)^m$$

gives a order s method.

<u>Check</u>

$$\rho(\omega) - \ln \omega \cdot \sigma(\omega) = \beta \sum_{m=1}^{s} \frac{1}{m} \omega^{s-m} (\omega - 1)^m - \beta \omega^s \ln \omega$$

// <u>In the book.</u>

$$= O\left(|\omega - 1|^{s+1}\right)$$

$$\rho(\omega) = \beta\left\{\frac{1}{1}\cdot\omega^s + \frac{1}{2}\cdot\omega^s + \cdots + \frac{1}{s}\omega^s\right\}$$ (1')

$$+ A\omega^{s-1} + B\omega^{s-2} + \cdots$$

$$= \beta\sum_{m=1}^{s}\frac{1}{m}\,\omega^s + \cdots$$

set $\beta = 1/\sum \frac{1}{m}$

<u>Thm</u> A BDF obeys the root condition, and is convergent iff $1 \le s \le 6$.
(all listed p. 494 S&B)

<u>$s = 2$</u>

$$y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n = \frac{2}{3}h\,f(y_{n+2}, t_{n+2})$$

<u>$s = 3$</u>

$$y_{n+3} - \frac{18}{11}y_{n+2} + \frac{9}{11}y_{n+1} - \frac{2}{11}y_n = \frac{6h}{11}f(y_{n+3}, t_{n+3})$$

$$\ln \omega = \sum_{m=1}^{s} \frac{(-1)^{m+1}}{m} \xi^{m}, \quad \xi = \omega - 1$$

$$\beta \sum_{m=1}^{s} \frac{1}{m} [$$

Stiff ODEs

$$u_t = u_{xx} \qquad u(x,0) = \sin(\cos x)$$

Note: $\hat{u}_{0,k}$ decays exponentially fast for $k >> 1$.

Evolve the PDE forward as a set of ODE's for the Fourier amplitudes

$$\frac{d}{dt}\hat{u}_k = -k^2 \hat{u} \quad ; \quad |k| < N/2$$

$$\Rightarrow \hat{u}_k = \hat{u}_{k,0} e^{-k^2 t} \sim e^{-|k| g} e^{-k^2 t}$$

$k >> 1$.

Large wave number components contribute little to the solution, but can govern the stability of numerical schemes for integration.

$$\hat{u}_{k,n+1} = \hat{u}_{k,n} - \Delta t \, k^2 \hat{u}_{k,n} = (1 - \Delta t \, k^2)\hat{u}_{k,n}$$

$$= (1 - \Delta t \, k^2)^{n+1} \hat{u}_{k,0}$$

If $\dot{y} = Ay$, $A = P\Lambda P^{-1}$

$$P^{-1}\dot{y} = \Lambda P^{-1} y \Rightarrow z_t = \Lambda z$$

Most ~~the~~ rapidly decaying mode, or most negative e.v. of A will control numerical stability.

13

A necessary condition for convergence to "true" solution is that

$$\underbrace{-1 \le 1 - \Delta t\, k^2} \le 1$$

$\Rightarrow$ $\Delta t \le 1/k^2$; called a stability condition & must be satisfied $\forall\, k$. $\Delta t < 1/N^2$.

<u>Note</u> stability condition dictated by those modes that decay the fastest & contribute the least to the solution

---

<u>Backward Euler</u>

$$\hat{u}_{k,n} = \frac{1}{(1+\Delta t k^2)^n}\, \hat{u}_{k,0}$$

Always satisfies stability condition but is of low-order.

<u>Trapezoidal</u> $\hat{u}_{k,n+1} = \hat{u}_{k,n} - \Delta t\, k^2 \frac{1}{2}\left(\hat{u}_{k,n+1} + \hat{u}_{k,n}\right)$

$\Rightarrow$ $\hat{u}_{k,n} = \left(\dfrac{1 - \frac{1}{2}\Delta t k^2}{1 + \frac{1}{2}\Delta t k^2}\right)^n \hat{u}_{k,0}$ | stable & 2^{nd}-order.

$\dfrac{1-a}{1+a} < 1$ for any $a > 0$.

A - stability

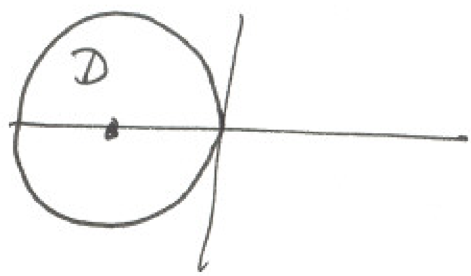
Consider $\frac{dy}{dt} = \lambda y \quad t \geq 0,\ y(0) = 1,\ \lambda \in \mathbb{C}$

$$y(t) = e^{\lambda t} \Rightarrow \left[\lim_{t\to\infty} y(t) = 0 \Leftrightarrow \mathrm{Re}\,\lambda < 0 \right]$$

__Defn__ The __linear__ __stability__ domain D of a numerical method for evolving y is the set of $\lambda \cdot h \in \mathbb{C}$ s.t. $\lim_{n\to\infty} y_n = 0$

__Euler__ $\quad y_n = (1+h\lambda)^n$

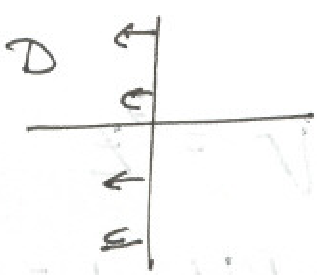
$$D = \{ z \mid |1+z| < 1 \}$$



__Trapezoidal__

$$D = \left\{ z \;\middle|\; \left| \frac{1+\frac{1}{2}z}{1-\frac{1}{2}z} \right| < 1 \right\} = \{ z \mid \mathrm{Re}\, z < 0 \} = \mathbb{C}^-$$

which mimics the stability properties of the ODE.



$$\vec{y}_t = \underline{\underline{A}}\, \underline{\underline{y}} \qquad A = P \Lambda P^{-1} \qquad AP = P\underline{\Lambda}$$

$$= P \Lambda P^{-1} y \Rightarrow Z_t = \underline{\Lambda} z, \quad z = P^{-1} y$$

Again

Defn A method is called *A-stable* if $\mathbb{C}^{-1} \subseteq D$.

RK2
$$y_{n+1} = y_n + h\tfrac{1}{2}(k_1 + k_2)$$
$$k_1 = f(y_n, t_n) = \lambda y_n$$
$$k_2 = f(y_n + h f(y_n, t_n), t_{n+1})$$
$$= \lambda(y_n + h\lambda y_n)$$

$$y_{n+1} = y_n + \tfrac{1}{2} h\lambda (2y_n + h\lambda y_n)$$
$$= \left(1 + h\lambda + \tfrac{1}{2}(h\lambda)^2\right) y_n$$

$$D = \left\{ z \,\middle|\, |1 + z + \tfrac{1}{2}z^2| < 1 \right\} = \left\{ z \,\middle|\, |z^2 + 2z + 2| < 2 \right\}$$

$(z+1)^2 + 1$

$R^2 e^{2i\theta} + 1$

Not A-stable

Unbded in the left half-plane, hence is not A-stable.

Indeed, no explicit RK scheme is A-stable.

Thm The Gauss-Legendre IRK methods (ν stage, 2ν order) are A-stable.

Multi-step applied to $\dot{y} = \lambda y$

Write as $\displaystyle\sum_{m=0}^{s} \underbrace{(a_m - h\lambda b_m)}_{g_m} y_{n+m} = 0$

Again, a linear difference eqn.

Characteristic polynomial:

$$\sum_{m=0}^{s} g_m \omega^m$$

Has generally, q zeroes $\omega_1, \ldots, \omega_q$ w. resp. multiplicities $k_1, \ldots, k_q$, where $\displaystyle\sum_{m=0}^{q} k_m = s$

Solutions can be represented as

$$y_n = \sum_{i=1}^{q} \left[\sum_{j=0}^{k_i - 1} c_{ij} n^j \right] \omega_i^n$$

$\underline{k_i > 1}$ ⇒ algebraic part of growth due to higher multiplicity.

Constants c_{ij} (of which there are s) are determined by initial data $y_0, \ldots, y_{s-1}$

Hence, the zeroes of $\sum g_m \omega^m$ will govern the A-stability.

<u>Thm</u> Let $w_1(z), \dots, w_{g(z)}(z)$ be the zeroes of

$$\eta(z,\omega) = \sum_{m=0}^{s} (a_m - z b_m)\,\omega^m, \quad z \in \mathbb{C}$$

The method is A-stable <u>iff</u>

$$|w_i(z)| < 1, \quad i = 1, \dots, g(z) \quad \forall\, z \in \mathbb{C}^-$$

<u>Pf.</u> Elementary, in text.

<u>Comments</u>

~~AB methods~~

1.) For ~~AB methods~~ Adams methods, the region of linear stability tends to shrink w increasing order s.

2.) Adams-Moulton (Adams method w. $b_s \neq 0$, i.e. implicit) tend to have larger lin. stability regions than AB methods.

3.) $b_s \neq 0$ is a <u>necessary</u> condition for A-stability.

4.) BDF methods have generous lin. stability regimes & the $s = 1, 2$ cases are A-stable, but

5.) (The Dahlquist 2^{nd} Barrier)

The highest order of an A-stable multi-step method is 2.

6.) Consider the Forward / Backward Euler method

$$y_{n+1} = y_n + h f(y_{n+1}, t_{n+1})$$

$$y_{n+2} = y_{n+1} + h f(y_{n+1}, t_{n+1})$$

How accurate is it? A-stability?

7.) In practical problems, methods are often mixed so as to achieve efficiency & accuracy & stability:

$$\frac{du}{dt} = \underbrace{f(u)}_{\text{lower order nonlinearity.}} + \underbrace{\nu g(u)}_{\text{linear operator w. high derivatives.}}$$

lower order nonlinearity. linear operator w. high derivatives. ~~Governs~~ Dominates. the lin. stability

<u>Mixed Method</u> $\qquad u_t + uu_x = \nu u_{xx}$

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{3}{2} f(u^n) - \frac{1}{2} f(u^{n-1}) \qquad \underline{AB2}$$

$$+ \frac{\nu}{2}\left[g(u^{n+1}) + g(u^n)\right] \qquad \text{trapez. rule.}$$

$$\Rightarrow \underbrace{u^{n+1} + \frac{\Delta t \nu}{2} g(u^{n+1})}_{\text{System of Linear Eqns.}} = R(u^n, u^{n-1})$$

System of Linear Eqns.

Don't require Newton's Method.

There are similar, higher-order BDF type schemes.

Other issues

1.) Special systems

- I & F systems
- DAE equations ; i.e. eqns with mixed differential/algebraic equations.

$$\begin{cases} X_t = \partial_s (T X_s) + F(x) \\ \text{to } X_s \cdot X_s = 1 \end{cases}$$

- Hamiltonian systems

$$\dot{p} = \frac{\partial H}{\partial q} p \qquad H = H[p,q]$$

$$\dot{q} = -\frac{\partial H}{\partial p}$$

$$\frac{d}{dt} H = H_p \dot{p} + H_q \dot{q} = H_p H_q - H_q H_p = 0$$

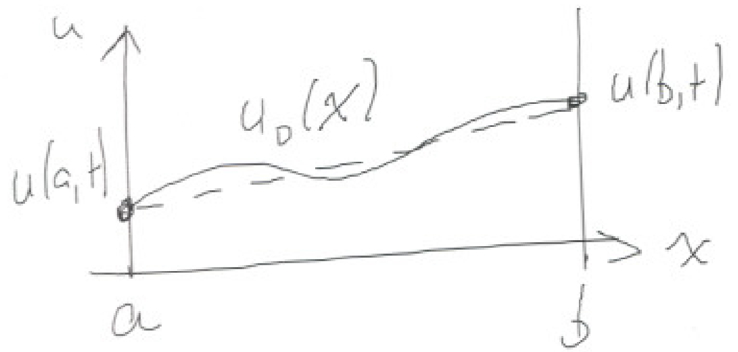
~~Conservation~~

Invariances are very important to understanding dynamics.

3 Fundamental PDEs

(1) $\dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2}$; the heat diffusion eqn. "parabolic"

Evolutionary, solved as an initial/boundary value problem



Specify initial data $u_0(x)$ for $x \in (a,b)$

and the boundary values $u(a,t)$ & $u(b,t)$

(the "Dirichlet problem")

Neumann problem: specify $u_x(a,t)$ & $u_x(b,t)$

$\dfrac{\partial u}{\partial t} = \nu \dfrac{\partial^2 u}{\partial x^2}$ "Well-posed" for $\nu > 0$

"Ill-posed" for $\nu < 0$ (backward diffusion)

Here well-posed if $\exists\ C > 0$ s.t.

$\|u\| \le C \|u_0\|$

use on next page.

Assume $u(a,t) = u(b,t) = 0$ | or rapid decay on the line $\mathbb{R}$.

Energy $\mathcal{E} = \frac{1}{2}\int_a^b u^2\,dx$

$$\dot{\mathcal{E}} = \int_a^b u\,u_t = \int_a^b u\,u_{xx}$$

$$= u\,u_x\Big|_a^b - \int_a^b u_x^2$$

$$= -\int_a^b u_x^2$$ // "Energy" decays via diffusion

If $u(a,t) = u_1$, $u(b,t) = u_2$, constants

Let

$$v = u - \underbrace{\left[u_1 \frac{x-b}{a-b} + u_2 \frac{x-a}{b-a}\right]}_{\text{asymptotic soln in time}}$$

$$\mathcal{E} = \tfrac{1}{2}\int v^2, \quad \dot{\mathcal{E}} \le 0.$$

Variants

High dimension.

(i.) $\frac{\partial u}{\partial t} = \Delta u$, $u : \mathbb{R}^n \times \mathbb{R}^+ \to \mathbb{R}^n$

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2}$$

(ii) $$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \underbrace{f(x,t)}_{\text{a "forcing term"}}$$

(iii) $$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[a(x)\frac{\partial u}{\partial x}\right] ; \quad a > 0$$

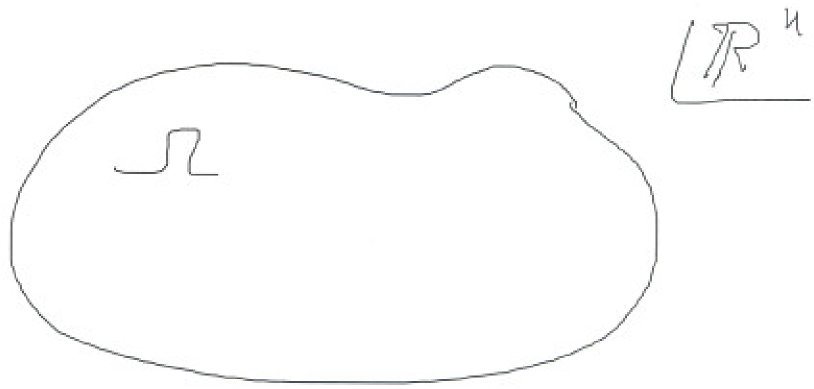
"a" – variable coefficient diffusion.

12) $\Delta u = f(\underline{x})$; The Poisson eqn. ("elliptic")

$\underset{\rightarrow}{x} \in \mathbb{R}^n$, $f : \mathbb{R}^n \to \mathbb{R}$

$\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$

Solved as a <u>boundary</u> <u>value problem</u> for u.



Solve $\Delta u = f$ for $\underline{x} \in \Omega$

$$\underbrace{\underbrace{\text{with } u\Big|_{\partial\Omega} = v(\underset{\rightarrow}{x}); \text{ Dirichlet}}_{} \quad \text{or} \quad \frac{\partial u}{\partial n} = \hat{n} \cdot \nabla_x u\Big|_{\Omega} = v(x) \text{ Neumann}}_{\text{The boundary values}}$$

Ill-posed as an IVP: $u_{xx} = -u_{yy}$

$w = u_x \Rightarrow w_x = -u_{yy}$ $\Big\|$ $(u, w) = \sum (\hat{u}, \hat{w}) e^{iky}$

$u_x = w$ $\qquad \hat{w}_x = k^2 \hat{u}$

Assume $\exists\, C$. Then $\exists\, k$ suff'ly large $\qquad \hat{u}_x = \hat{w}$

s.t. $\left\| \begin{pmatrix} u \\ w \end{pmatrix} \right\| > C \left\| \begin{pmatrix} u_0 \\ w_0 \end{pmatrix} \right\|$

Variants

(i.) $\Delta u = 0$ – Laplace's equation

(ii.) $\nabla \cdot \left(a(\underline{x}) \nabla u \right) = f(\underline{x})$

variable coefficient

(iii) $\Delta u + \alpha u = f$

$\alpha > 0$ – Helmholtz eqn.

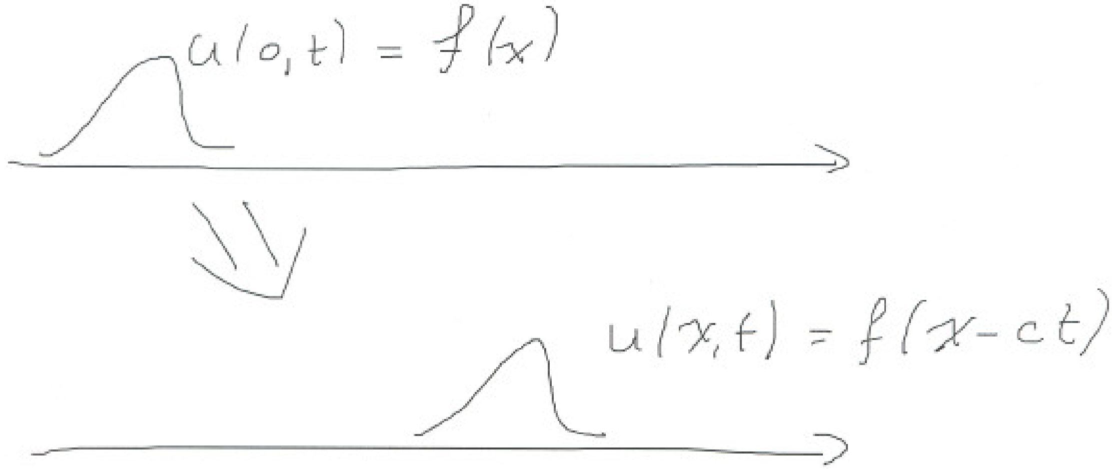
$\alpha < 0$ – "damped" elliptic.

(3) Hyperbolic

$u_t + c u_x = 0$ — One way wave eqn. $c > 0$; speed

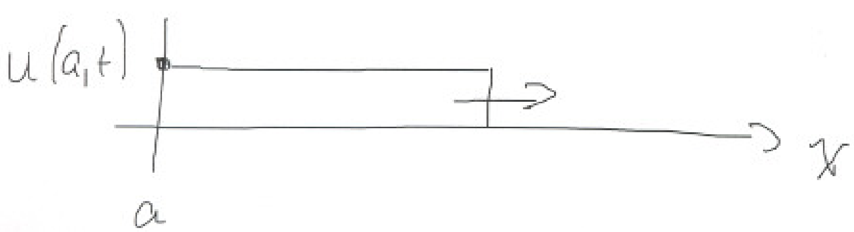
Evolutionary. Solved as initial value problems w. appropriate bdy value data.

Exact solution $u(x,t) = f(x - ct)$



Dir'l propagation of information.

Here, propagation is from left to right, so if there is a left bdy, can specify data there



Ill-posed here if data is posed at right end of domain.

Variants

(i) The wave equation – 2 dirns of info. propagation.

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0 = (\partial_t - c\,\partial_x)(\partial_t + c\,\partial_x)u$$

D'Alembert's solution: $u = f(x-ct) + g(x+ct)$
Decomposition into left & right travelling fns.

(ii) $$\frac{\partial^2 u}{\partial t^2} - \nabla\cdot\Big(\underbrace{c^2(x)}_{\text{variable speed}}\nabla u\Big) = \underbrace{f(\underline{x}, t)}_{\text{forcing term}}$$

(iii) $$\frac{\partial u}{\partial t} + \partial_x\Big[\underbrace{f(u)}_{\text{"flux"}}\Big] = 0$$

e.g. Nonlinear wave eqn

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

or $$\frac{\partial u}{\partial t} + \partial_x\Big(\underbrace{\tfrac{1}{2}u^2}_{\text{flux}}\Big) = 0$$

solve by method of characteristics.

<u>Example</u> The Navier-Stokes Eqn

$$\frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla) u = -\nabla p + \Delta \underline{u}$$

$$\nabla \cdot \underline{u} = 0$$

$$\underline{x}, u \in \mathbb{R}^{2 \text{ or } 3}$$

The N-S Eqs has parabolic, elliptic & hyperbolic aspects

$$\left(\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \nabla \underline{u} \right)_i = \underbrace{\frac{\partial u_i}{\partial t} + \sum_j u_j \frac{\partial}{\partial x_j} u_i}_{\text{Hyperbolic type operator}}$$

$$\frac{\partial \underline{u}}{\partial t} + N = \Delta u \quad \text{parabolic.}$$

$$\nabla \cdot u = 0, \quad \nabla \cdot u_t = 0, \quad \nabla \cdot (\Delta u) = \Delta (\nabla \cdot u) = 0$$

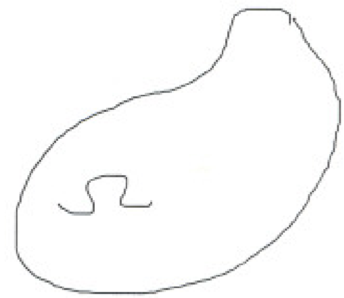
$$\Rightarrow \quad \Delta p = -\nabla \cdot [(\underline{u} \cdot \nabla) u]$$

elliptic

Example – Implicit-in-time differencing of the heat diffusion eqn:

$$\frac{\partial u}{\partial t} = \Delta u + f$$

in Ω



with initial data $u_0(\underline{x})$ and bdy values $u(x,t)\big|_{\partial\Omega} = v(x)$

$$u_{n+1} = u_n + \Delta t \cdot \left[\Delta u_{n+1} + f(\underline{x}, t_{n+1})\right]$$

(Better: $u_{n+1} = u_n + \frac{\Delta t}{2}\left[(\Delta u_{n+1} + \Delta u_n) + (f_n + f_{n+1})\right]$

$$\Rightarrow \quad \Delta u_{n+1} - \frac{1}{\Delta t} u_{n+1} = -\frac{1}{\Delta t} u_n - f_n$$

<u>or</u> $\quad \Delta v - \alpha v = g$

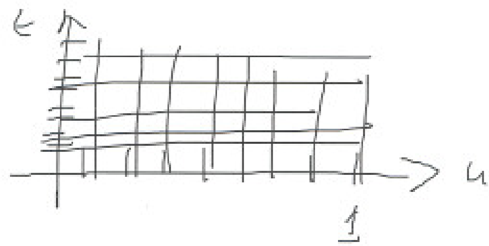
A damped Poisson eqn.

The diffusion equation

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

evolved on the strip $S = \{(x,t) \mid x \in [0,1], t \geq 0\}$

Discretize with a uniform grid in both x & t:



$u_j^n \simeq u(j\Delta x, n\Delta t)$

$$\{(j\Delta x, n\Delta t) \mid j = 0(1)N,\ n \geq 0\}$$

$$\Delta x = 1/N, \quad \Delta t = T/M$$

Replace $\frac{\partial u}{\partial t}$ by a forward difference

and $\frac{\partial^2 u}{\partial x^2}$ by a centered difference

& consider Euler's Method:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

$$\Rightarrow \quad u_j^{n+1} = u_j^n + \mu \left[u_{j+1}^n - 2u_j^n + u_{j-1}^n \right]$$

$$\mu = \frac{\Delta t}{\Delta x^2} = \text{Courent Number}$$

Initial & Bdy Data

$$\begin{cases} u_j^0 = v(j \cdot \Delta x) \\ u_0^n = g_0(n \cdot \Delta t), \quad u_N^n = g_1(n \cdot \Delta t) \end{cases}$$

Accuracy Substitute true soln into differenced equation

$$\frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} - \frac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{\Delta x^2}$$

$$= O(\Delta t, \Delta x^2)$$

$\downarrow$

Set $\mu = \frac{\Delta t}{\Delta x^2}$ constant

$\downarrow$

$$= O(\Delta x^2)$$

Convergence

Method called convergent if for any $T>0$ ~~$t>0$~~

$$\lim_{\Delta x \downarrow 0}\left\{\lim_{j\to x/\Delta x}\ \lim_{n\to t/\Delta t} u_j^n\right\} = u(x,t)$$

$$\forall\, x,t \in S'$$

Thm If $\mu \le 1/2$, then the above method is convergent.

Pf. Similar to that for E.M. in ODE.

Fix $T>0$. Define $e_j^n = u_j^n - u(j\cdot\Delta x, n\cdot\Delta t)$

for $j = 0(1)N$, $n = 0(1)\,n_{\Delta t}$

where $n_{\Delta t} = T/\Delta t = T/(\mu\Delta x^2)$

Convergence:

$$\lim_{\Delta x\to 0}\left\{\max_{j=0(1)N}\ \max_{n=0(1)n_{\Delta t}} |e_j^n|\right\} = 0$$

Let $\eta_n = \max_{j=0(1)N} |e_j^n|$

$$\Rightarrow \lim_{\Delta x \to 0} \max_{n=0(1)n_{\Delta t}} \eta_n = 0$$

$$u_j^{n+1} = u_j^n + \mu \left[u_{j+1}^n - 2u_j^n + u_{j-1}^n \right]$$

Let $\tilde{u}_j^n = u(j\Delta x, n\Delta t)$

Then:

$$\frac{\tilde{u}_j^{n+1} - \tilde{u}_j^n}{\Delta t} - \frac{\tilde{u}_{j+1}^n - 2\tilde{u}_j^n + \tilde{u}_{j-1}^n}{\Delta x^2} = \mathcal{O}(\Delta x^2, \Delta t)$$

μ fixed $\Rightarrow$
+ smoothness

$$\tilde{u}_j^{n+1} = \tilde{u}_j^n + \mu \left[\tilde{u}_{j+1}^n - 2\tilde{u}_j^n + \tilde{u}_{j-1}^n \right] + \mathcal{O}(\Delta x^4)$$

$$\Rightarrow e_j^{n+1} = e_j^n + \mu \left[e_{j+1}^n - 2e_j^n + e_{j-1}^n \right] + \mathcal{O}(\Delta x^4)$$

$$\Rightarrow |e_j^{n+1}| \le \mu |e_{j-1}^n| + |1 - 2\mu| \cdot |e_j^n| + \mu |e_{j+1}^n| + C \cdot \Delta x^4$$

$$\le \left[2\mu + |1 - 2\mu| \right] \eta^n + C \cdot \Delta x^4$$

$\mu \le 1/2 \Rightarrow 2\mu + |1-2\mu| = 1$

$\Rightarrow \eta^{n+1} \le \eta^{n} + C' \Delta x^4$

$\Rightarrow \eta^{n+1} - \eta^{n} \le C' \Delta x^4$

$\Rightarrow \sum_{k=0}^{n} \eta^{k+1} - \eta^{k} \le C' \cdot (n+1) \cdot \Delta x^4$

$\Rightarrow \eta^{n} \le C' \cdot n \cdot \Delta x^4 + \eta^{0}$

$\eta^{0} = 0$

Note! $n \cdot \Delta x^2 = n \cdot \Delta t / \mu = t_n / \mu$

$\Rightarrow \eta^{n} < C' t_n \cdot \Delta x^2 = C' \cdot T \cdot \Delta x^2$ ✓

Add'l comments:

2^{nd}-order convergence in Δx, where $\Delta t \sim \Delta x^2$.

This is the stability condition associated with A-stability in a method of lines treatment

Implicit Methods allow Δt & Δx to be taken to zero independently

Crank - Nicholson $\qquad u_t = u_{xx}$

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}\left[D_x^2 u^n + D_x^2 u^{n+1} \right]$$

$$u_j^{n+1} - \frac{\Delta t}{2\Delta x^2}\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} \right) = R_j^n$$

$$u_0^{n+1} = a \ , \quad u_{N+1}^{n+1} = b$$

$$\begin{pmatrix} 1 + \frac{\Delta t}{\Delta x^2} & -\frac{1}{2}\frac{\Delta t}{\Delta x^2} & 0 \\ -\frac{1}{2}\frac{\Delta t}{\Delta x^2} & 1 + \frac{\Delta t}{\Delta x^2} & -\frac{1}{2}\frac{\Delta t}{\Delta x^2} \\ & \ddots & \ddots \\ 0 & -\frac{1}{2}\frac{\Delta t}{\Delta x^2} & 1 + \frac{\Delta t}{\Delta x^2} \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_N^{n+1} \end{pmatrix} = \underline{R}$$

tridiagonal system $O(N)$ solve for each time-step.

$O(\Delta t^2, h^2)$ accuracy

[illegible]

Periodic B.C.'s.

$$u_t = N(u) + u_{xx}$$

Use C-N or Integrating-Factor methods.

$$u_j = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{u}_k e^{ijkh}$$

$$(D^2 u)_j = -\sum_k k^2 \hat{u}_k e^{ijkh}$$

$$\frac{d}{dt}\hat{u}_k = \widehat{N(u)}_k - k^2 \hat{u}_k \qquad |k| \le \frac{N}{2}$$

Go over integrating factor.

$$O(N \ln N)$$

$\cancel{O(\Delta t^2)}$, Highly accurate.

$$\frac{d}{dt}\Big(\underbrace{e^{k^2 t}\hat{u}_k}_{\psi}\Big) = e^{k^2 t}\hat{N}_k$$

$$\frac{\psi^{n+1} - \psi^{n}}{\Delta t} = \frac{1}{2}\left[3e^{k^2 t_n}\hat{N}_k^{n} - e^{k^2 t_{n-1}} N_k^{n-1}\right]$$

$$\frac{e^{k^2 t_{n+1}}\hat{u}_k^{n+1} - e^{k^2 t_n}\hat{u}_k^{n}}{\Delta t} = \frac{1}{2}\left[3e^{k^2 t_n}\hat{N}_k^{n} - e^{k^2 t_{n-1}}\hat{N}_k^{n-1}\right]$$

$$\hat{u}_k^{n+1} = e^{-k^2\Delta t}\hat{u}_k^{n} + \frac{1}{2}\left[3e^{-k^2\Delta t}\hat{N}_k^{n} - e^{-2k^2\Delta t}\hat{N}_k^{n-1}\right].$$

<u>Very stable.</u>

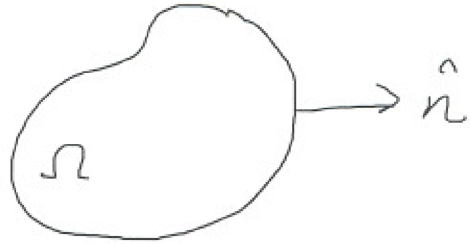
Higher Dimension

$$\frac{u^{n+1} - u^{n-1}}{2\Delta t} = \cancel{A}(u^n) + \frac{1}{2}\left(\Delta u^{n+1} + \Delta u^{n-1}\right)$$

$$\frac{1}{\Delta t} u^{n+1} - \Delta u^{n+1} = R$$

Elliptic problem.

Poisson Eqn
in a closed
simply-connected
domain Ω



$$\Delta u = f \text{ in } \Omega$$
$$u = g \text{ on } \partial\Omega$$

f, g smooth

<u>Thm</u> $\exists A$! smooth u ~~exists~~

Uniqueness - Assume two solutions

u & v $\Rightarrow$ $r = u - v$ satisfies

$$\Delta r = 0 \text{ in } \Omega$$
$$r = 0 \text{ on } \partial\Omega$$

$$\int_\Omega |\nabla r|^2 = \int_\Omega \nabla \cdot (r \nabla r) - \underbrace{\int r \Delta r}_{=0}$$

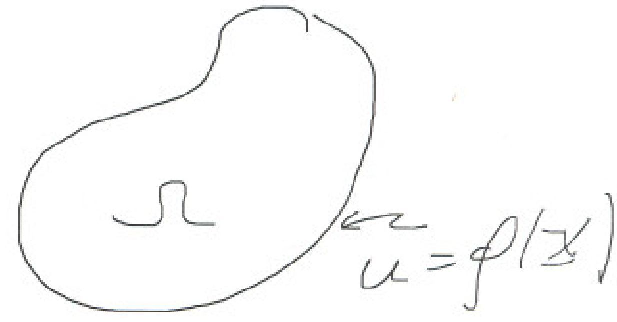
$$= \int_{\partial\Omega} r \frac{\partial r}{\partial n} = 0$$

$\Rightarrow$ $\nabla r = 0$ $\Rightarrow$ $r = \text{Const}$

$r|_{\partial\Omega} = 0 \Rightarrow r = 0 \Rightarrow$ $\boxed{u = v}$

Poisson's Equation

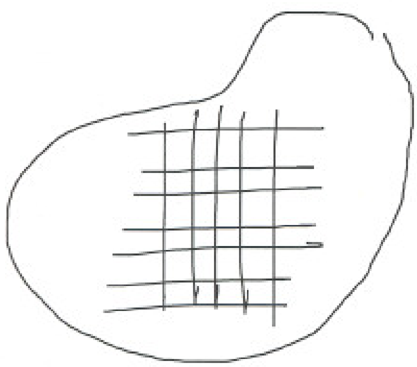
$$(1)\begin{cases} \nabla^2 u = f \quad \text{in } \Omega \\ u\Big|_{\underline{x}\in\partial\Omega} = g(x) \end{cases}$$



Consider $d = 2$, $\nabla^2 u = \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial y^2} u$

Common approach: Replace u_{xx} & u_{yy} by centered differences on a square grid

Grid points $(x_0 + kh, y_0 + lh)$, $k, l \in \mathbb{Z}$

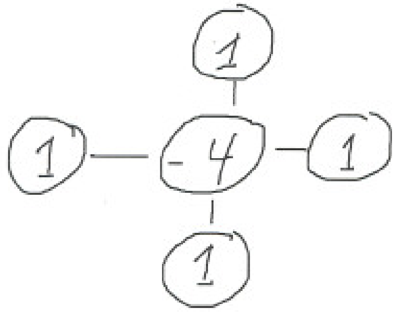


Replace $\nabla^2 u = f$ with

$$\frac{u_{k+1,l} - 2u_{k,l} + u_{k-1,l}}{h^2} + \frac{u_{k,l+1} - 2u_{k,l} + u_{k,l-1}}{h^2} = f_{k,l}$$

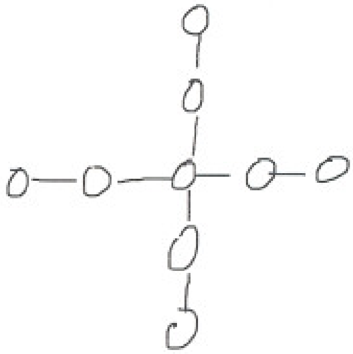
24) There are higher order approaches

2nd - order



$u_{kl} = h^2 f_{kl}$

(I) Increase the order of the approx. to ∂_{xx} & ∂_{yy}

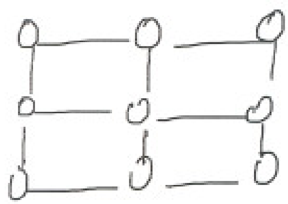
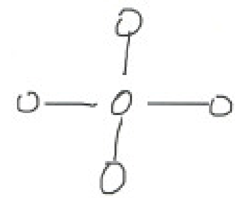


$u_{k,l} = h^2 f_{k,l}$

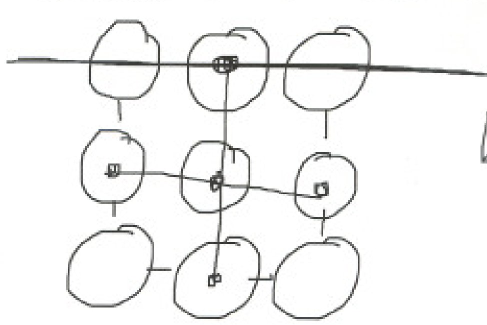
A 9-point stencil

Not so nice w. bdy data

(II) Use a more compact stencil

 $u_{k,l} = h^2$  $f_{k,l}$

4th-order & interacts nicely w. bdy (upon which f is assumed known)



bdy stencil

Set $\underline{y}_\ell = \underline{\underline{Q}}\, \underline{x}_\ell$, $c_\ell = \underline{\underline{Q}}\, b_\ell$

$\Rightarrow$

$$y_{\ell-1} + \underline{\underline{D}}\, y_\ell + y_{\ell+1} = c_\ell$$

$$\begin{bmatrix} D & I & & \\ I & D & I & \\ & I & D & I \\ & & I & D \end{bmatrix} \begin{bmatrix} \underline{y}_1 \\ \underline{y}_2 \\ \vdots \\ \underline{y}_{N_2} \end{bmatrix} = \begin{bmatrix} \underline{c}_1 \\ \underline{c}_2 \\ \vdots \\ c_{N_2} \end{bmatrix}$$

Before proceeding, how expensive is it to evaluate the transformations

$\cancel{\underline{\underline{Q}}\, \underline{x}_\ell,\ x\, f}$ $\quad \underline{\underline{Q}}\, \underline{b}_\ell$? $\quad \underline{\underline{Q}} \in \mathbb{R}^{N_1 \times N_1}$

First answer: $O(N_1^2)$, but

$$c_k = \sum_{k=1}^{N_1} q_{jk}\, b_k = \left(\frac{2}{N_1+1}\right)^{1/2} \left(\sum_{k=1}^{N_1} b_k \sin\left(\frac{\pi j k}{N_1+1}\right)\right)$$

This is a sine transform, a special case of the DFT.

This can be evaluated via FFT

in $O(N_1 \ln N_1)$ operations

$$\Rightarrow \quad \underline{x}_{l-1} + \underline{\underline{S}}\,\underline{x}_l + \underline{x}_{l+1} = \underline{b}_l \,; \quad l = 1(1)N_2$$

w. $\quad \underline{x}_0 = \underline{x}_{N_2+1} = \underline{0}$

$\underline{\underline{S}}$ is a tridiagonal, symmetric Toeplitz matrix (see p. 197 of Iserles)

$$\underline{\underline{S}} = \begin{pmatrix} \alpha & \beta & & & \\ \beta & \alpha & \beta & & \\ & \beta & \alpha & \beta & \\ & & \ddots & \ddots & \ddots \\ & & & \beta & \alpha \end{pmatrix}$$

The eigenvectors of $\underline{\underline{S}}$ are known

$$\underline{\underline{S}} = \underline{\underline{Q}}\,\underline{\underline{D}}\,\underline{\underline{Q}} \quad ; \quad \underline{\underline{Q}} \text{ orthogonal}$$

w $\underline{\underline{D}}$ diagonal, $D_{ii} = \lambda_i$ = eigenvalue of $\underline{\underline{S}}$

$$q_{jl} = \left(\frac{2}{N_1+1}\right)^{1/2} \cdot \sin\left(\frac{\pi j l}{N_1+1}\right)$$

$\Rightarrow \quad \underline{\underline{Q}}$ symmetric.

$$\lambda_j = \alpha + 2\beta \cos\frac{\pi j}{N_1+1} = -4 + 2\cos\frac{\pi j}{N_1+1}$$

More closely $N_1 = 2$, $N_2 = 3$

$$\left(\begin{array}{cc|cc|cc} \lambda_1 & 0 & 1 & 0 & & \\ 0 & \lambda_2 & 0 & 1 & \multicolumn{2}{c}{0} \\ \hline 1 & 0 & \lambda_1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \lambda_2 & 0 & 1 \\ \hline & & 1 & 0 & \lambda_1 & 0 \\ \multicolumn{2}{c|}{0} & 0 & 1 & 0 & \lambda_2 \end{array}\right) \left(\begin{array}{c} y_{11} \\ y_{21} \\ \hline y_{12} \\ y_{22} \\ \hline y_{13} \\ y_{33} \end{array}\right) = \underset{\to}{c}$$

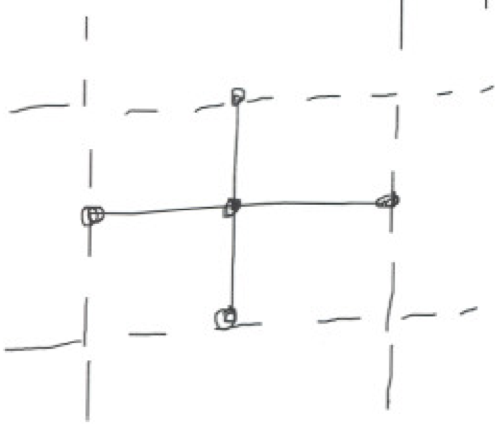
Re-order $y_e \to \tilde{y}_i$, $\tilde{y} = \left(\begin{array}{c} y_{11} \\ y_{12} \\ y_{13} \\ \hline y_{21} \\ y_{22} \\ y_{23} \end{array}\right)$

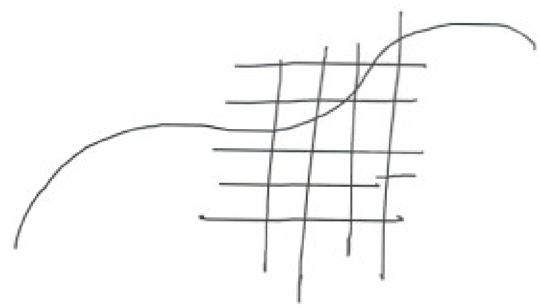
$$\left(\begin{array}{ccc|ccc} \lambda_1 & 1 & 0 & & & \\ 1 & \lambda_1 & 1 & & 0 & \\ 0 & 1 & \lambda_1 & & & \\ \hline & & & \lambda_2 & 1 & 0 \\ & & & 1 & \lambda_2 & 1 \\ & & & 0 & 1 & \lambda_2 \end{array}\right) \left(\begin{array}{c} \tilde{y}_1 \\ \\ \underset{\to}{\tilde{y}}_2 \end{array}\right) = \tilde{c}$$

System decouples into tridiagonal systems.

or
$$u_{k+1,l} + u_{k-1,l} + u_{k,l+1} + u_{k,l-1} - 4u_{k,l}$$
$$= h^2 f_{k,l}$$

Called the five-point stencil:





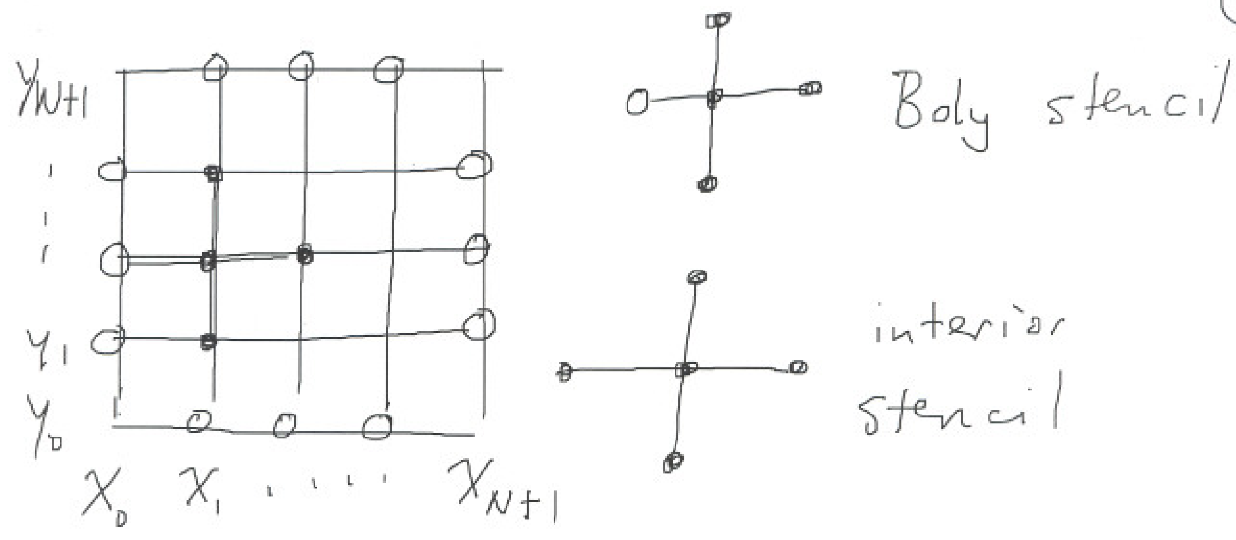
This approximation is intended only for the interior of the set.

Q: What should be done at the bdy?

How is bdy data applied?

Make it easier: Let Ω be the unit square $0 \le x, y \le 1$, and ~~let~~ take the grid points

(kh, lh), $h = 1/(N+1)$, $(k,l) = 1(1)N$



Now grid pts sit in interior and on the body. Application of body data is now trivial

This yields N^2 linear eqns for N^2 unknowns.

Does a soln exist & is unique? Yes

How accurate is it? $O(h^2)$

How efficiently can it be solved?

$O(N^2 \ln N)$

20)

Let $\underset{\to}{u} = (u_{k_1 l_1}, u_{k_2 l_2}, \dots, u_{k_{N^2} l_{N^2}})^T$

& write system as

$$\underset{=}{A}\,\underset{\to}{u} = \underset{\to}{b}$$ where $\underset{\to}{b}$ contains values of $f_{k,l}$ & boundary data

Here $\underset{=}{A} \in \mathbb{R}^{N^2 \times N^2}$

<u>Lemma</u> $\underset{=}{A}$ is symmetric and has the set of eigenvalues

$$\lambda_{m,n} = -4\left[\sin^2 \frac{m\pi}{2(N+1)} + \sin^2 \frac{n\pi}{2(N+1)}\right]$$

$$m, n = 1(1)N$$

[<u>Note</u>: arguments of $\sin^2$ are never a multiple of $\pi \Rightarrow \lambda_{m,n} < 0$]

<u>Pf.</u> Symmetry - direct

20)

The vector

$$v_{kl} = \sin \frac{km\pi}{N+1} \sin \frac{ln\pi}{N+1}$$

$$k, l = 1(1)N$$

satisfies

$$v_{k-1,l} + v_{k+1,l} + v_{k,l+1} + v_{k,l-1} - 4v_{k,l}$$

$$= \lambda_{mn} v_{kl} \quad \checkmark$$

<u>Corollary</u> $\underline{\underline{A}}$ is negative definite & non singular

$\Rightarrow \exists!$ solution exists.

Let $e_{k,l} = U_{k,l} - u(kh, lh)$

$= U_{k,l} - \tilde{u}_{k,l}; \quad \underset{\rightarrow}{e} \in \mathbb{R}^{N^2}$

Let $\|\cdot\|$ denote the Euclidean norm.

$$\|\underset{\rightarrow}{e}\| = (e^T e)^{1/2} = \left[\sum_i e_i^2\right]^{1/2}$$

Let $\|\underset{\rightarrow}{e}\|_h = \left[h^2 \sum_i e_i^2\right]^{1/2}$

$$\simeq \left(\iint_\Omega E^2(x,y)\right)^{1/2} = \|E\|_2$$

<u>Theorem</u> Given f & g suff'ly smooth, $\exists$ $c > 0$ s.t. $\|e\|_h \leq c h^2$ as $h \to 0$.

<u>Pf.</u> $\tilde{u}_{k+1,l} + \tilde{u}_{k-1,l} + \tilde{u}_{k,l+1} + \tilde{u}_{k,l-1} - 4\tilde{u}_{k,l}$

$$= h^2 f_{k,l} + O(h^4)$$

$\Rightarrow e_{k+1,l} + e_{k-1,l} + e_{k,l+1} + e_{k,l-1} - 4e_{k,l} = O(h^4)$

$\Rightarrow \underline{\underline{A}}\, \underset{\rightarrow}{e} = \underline{\delta}_h$ with $\|\delta_h\|_h = O(h^4)$

$$\left[\|\delta_h\|_h \sim \left[h^2 \cdot N^2 \cdot (h^4)^2\right]^{1/2} \sim O(h^4)\right]$$

22)

$$\Rightarrow \quad \vec{e} = \underline{\underline{A}}^{-1} \vec{\delta}_h$$

$$\Rightarrow \quad \| \vec{e} \| \leq \| \underline{\underline{A}}^{-1} \| \cdot \| \vec{\delta}_h \|$$

$$\Rightarrow \quad \| \vec{e} \|_h \leq \| \underline{\underline{A}}^{-1} \| \cdot \| \vec{\delta}_h \|_h$$

Recall $\quad \rho(\underline{\underline{A}}) = \max \{ |\lambda| : \lambda \text{ e.v. of } \underline{\underline{A}} \}$

$\rho(A) \leq \| \underline{\underline{A}} \|$, $\| \cdot \|$ Euclidean

$\rho(A) = \| \underline{\underline{A}} \|$, for $\underline{\underline{A}}$ normall

$$A^T A = A A^T$$

Here $\underline{\underline{A}}$ is symmetric, hence normal

$\Rightarrow$ $\underline{\underline{A}}^{-1}$ is symmetric, hence normal

$$\Rightarrow \quad \| A^{-1} \| = \max |\lambda|^{-1} = \frac{1}{\min |\lambda|}$$

$$= \frac{1}{\min\limits_{m,n} 4 \left[\sin^2\left(\frac{m\pi}{2(N+1)} \right) + \sin^2\left(\frac{n\pi}{2(N+1)} \right) \right]}$$

$$= 1/8 \cdot \sin^2\left(\frac{h\pi}{2} \right)$$

$\Rightarrow$ For h suff'ly small, $\exists\ \tilde{c}$ s.t.

$$\|A^{-1}\| \leq c_1 h^{-2}$$ [sin αh behaves linearly near $h=0$]

$$\Rightarrow \|e\|_h \leq c h^{-2} \cdot h^4 = c h^2$$

Thus, the five point stencil yields a 2^{nd}-order solution.

Fast Poisson Solvers - Illustrate for 5-point

Use "natural" ordering

Let $\underset{\sim}{x}_\ell = \begin{bmatrix} u_{1,\ell} \\ \vdots \\ u_{N_1,\ell} \end{bmatrix}, \quad \underset{\sim}{b}_\ell = \begin{bmatrix} b_{1,\ell} \\ \vdots \\ b_{N_1,\ell} \end{bmatrix} \in \mathbb{R}^{N_1}$

solution along a column

for $\ell = 1(1)N_2$

$$\begin{bmatrix} S & I & & & 0 \\ I & S & I & & \\ & I & S & I & \\ & & & \ddots & \\ 0 & & & I & S \end{bmatrix} \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \vdots \\ \underline{x}_{N_2} \end{bmatrix} = \begin{bmatrix} \underline{b}_1 \\ \vdots \\ \vdots \\ b_{N_2} \end{bmatrix}$$

$I, S \in \mathbb{R}^{N_1 \times N_1}$

$$\underline{\underline{S}} = \begin{pmatrix} -4 & 1 & & & 0 \\ 1 & -4 & 1 & & \\ & 1 & -4 & 1 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & 1 & -4 \end{pmatrix}, \quad \underline{\underline{I}} = \text{identity}.$$

That is, the equation for $\underset{\sim}{y}$ can be re-ordered into N_1 decoupled, tridiagonal systems of size $N_2 \times N_2$.

$$\begin{pmatrix} \lambda_j & 1 & & \\ 1 & \lambda_j & 1 & \\ & \ddots & \ddots & \\ & & 1 & \lambda_j \end{pmatrix} \tilde{y}_j = \tilde{c}_j \qquad j = 1(1)N_1$$

Cost of solution : $\mathcal{O}(N_2)$ each.

<u>Algorithm</u> :

(1) For N_2 vectors $b_\ell \in \mathbb{R}^{N_1}$, form

$\underline{c}_\ell = \underline{\underline{Q}}\, b_\ell$. Cost $\mathcal{O}(N_2 N_1 \ln N_1)$

(2) Re-ording of $\underset{\sim}{y}$ is free of cost.

(3) Solve N_1 tridiagonal $N_2 \times N_2$ systems
Cost $\mathcal{O}(N_1 N_2)$

(4) Rearrange y at no cost.

(5) Form tf $\underset{\to}{x}_\ell = \underline{\underline{Q}}\, y_\ell$

Cost $\mathcal{O}(N_2 N_1 \ln N_1)$

- Can be applied to higher order stencil
- Can be applied to other equations, such as the biharmonic $\Delta^2 u = f$.
- Can be extended to $d = 3$.

It is not apparent how to apply this methodology beyond the square, or similarly simple domains

There has been interesting work in this direction by Mayo, Greengard, and co-workers. eg

A. Mayo – The fast solution of Poisson's and the biharmonic equation in irregular domains, SIAM J. Num. Anal. 21, p. 285 (1984)

What's not covered:

- Multi-grid
- FEM
- Bdy integral / integral methods.