Numerical Methods in Engineering
MSJ 1533

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Ordinary differential equations (ODEs)
Partial differential equations (PDEs)

Ordinary differential equations (ODEs)

First-order initial value problems : **single step methods**

Generally, *n*-order ODE has the form

$$\frac{d^n y}{dx^n} = y^{(n)} = f\left(x, y, y', y'', y^{(3)}, \cdots, y^{(n-1)}\right)$$

where *y* is function of single variable *x* and *n* is +ve integer.

If initial condition is given, $y(x=a)=y_0$, where *a* and y_0 are given constants, then it become **first-order initial value problem**.

Euler method

$$f(x+h) = f(x) + h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} + \cdots + h^n\frac{f^{(n)}(x)}{n!} + R_n^*.$$

Taylor's series at *x*=*a*

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n.$$

$$R_n = \frac{f^{(n+1)}(\theta x)}{(n+1)!}(x-a)^{n+1}, \quad a < \theta x < x.$$

Let $y=f$, $x_i=a$, $x_{i+1}=x$, $h=x-a$, and truncated the series after the second term, for $h\to 0$, we get

$$\boxed{y_{i+1} = y_i + hf(x_i, y_i) + O(h^2), \quad y_{i+1} \approx y_i + hf(x_i, y_i).}$$

Basic Euler formula, First order

Truncation error

"Big O" notation→$O(g(x))$.

Some finite value × $g(x)$

$O(h^2)$=Some finite value × h^2

$|O(h^2)| \le M|h^2|$

Definition: **$f(x)$ has order $O(g(x))$** as $x\to a$, if and only if **$|f(x)| \le M|g(x)|$** for $|x-a|<\delta$, where $0<M<\infty$, $\delta>0$.

Ordinary differential equations (ODEs)

First-order initial value problems : **single step methods**

Euler method

Example:

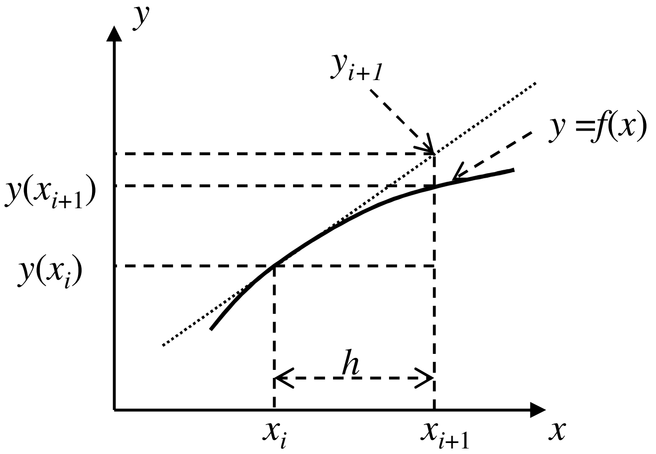
- if $f(x)=6x^4-2x^3$,

$f(x)$ has order $O(x^4)$ as $x\rightarrow\infty$, $f(x)$ has order $O(x^3)$ as $x\rightarrow 0$. $6x^4-2x^3+5$ has order O(1) as $x\rightarrow 0$.

- $(n+1)^2 = n^2 + O(n)+O(1)$.
- $(n+1)/n^2$ has order $O(1/n)$, $5/n+e^{-n}$ has order $O(1/n)$ as $n\rightarrow\infty$.

E.g. initial value problem:

$y'=y-t^2+1,\ 0 \le t \le 1,\ y(0)=0.5$



Let h =0.2, y_0=0.5, we get (here use 7 decimal places, D.P.)

$$\boxed{y_{i+1} = y_i + hf(t_i, y_i) = y_i + h(y_i - t_i^2 + 1), \quad i = 0,\cdots,4.}$$

dy/dt=$f(t,y)$

The exact solution is $y(t)=(t+1)^2-0.5e^t$.

Time, t_i	**Approx, y_i**	**Exact, $y(t_i)$**	**Absolute error, $\lvert y(t_i)-y_i\rvert$**
0.0	0.5	0.5	0
0.2	0.8	0.8292986	0.0292986
0.4	1.152	1.2140877	0.0620877
0.6	1.5504	1.6489406	0.0985406
0.8	1.98848	2.1272295	0.1387495
1.0	2.458176	2.6408591	0.1826831

- 48.4 & 48.0 have one **decimal place**
- 0.00001845, 0.0001845 and 0.001845 all have 4 **significant figures or digits**.
- 4.53×10^4, 4.530×10^4, 4.5300×10^4 have 3, 4 and 5 significant figures.

Ordinary differential equations (ODEs)

First-order initial value problems : **single step methods**

Improved Euler method – Heun's method

Slope ,$f(x,y)$, is the average of two derivatives.

$$y_i' = f(x_i, y_i) \rightarrow \quad y_{i+1}^0 = y_i + hf(x_i, y_i) \qquad\qquad y_{i+1}' = f\left(x_{i+1}, y_{i+1}^0\right)$$

Average slopes: $\bar{y}' = \dfrac{y_i' + y_{i+1}'}{2} = \dfrac{f(x_i, y_i) + f\left(x_{i+1}, y_{i+1}^0\right)}{2}$

Explicit form: $\boxed{y_{i+1} = y_i + \bar{y}'h = y_i + \dfrac{f(x_i, y_i) + f\left(x_{i+1}, y_{i+1}^0\right)}{2} h = y_i + \dfrac{h}{2}\left(f(x_i, y_i) + f(x_{i+1}, y_i + hf(x_i, y_i))\right)}$

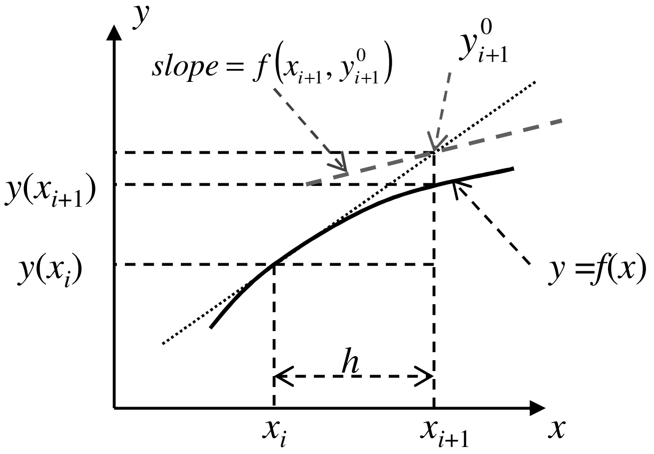
Predictor-corrector approach form:

Predictor: $y_{i+1}^0 = y_i + hf(x_i, y_i)$

Corrector: $y_{i+1} = y_i + \dfrac{f(x_i, y_i) + f\left(x_{i+1}, y_{i+1}^0\right)}{2} h$

$\underbrace{\hphantom{Predictor}}$

Predictor is basic Euler method



Ordinary differential equations (ODEs)

First-order initial value problems : **single step methods**

Improved Euler method – Heun's method

$y(x=1)=?$

E.g. **$y'=4e^{0.8x}-0.5y$**, $0\leq x\leq 4$, step size (h=1), initial condition, $y(0)=2$.

Analytical solution: $y=(4/1.3)[e^{0.8x}-e^{-0.5x}]+2e^{-0.5x}$

Standard Euler method

Slope at (x_0,y_0): $y_0' = 4e^0 - 0.5(2) = 3$ predictor→ $y_1^0 = y_0 + 1f(x_0, y_0) = 2 + 3(1) = 5$

(1 iteration) corrector→

$$y_1 = y_0 + \frac{f(x_0, y_0) + f(x_1, y_1^0)}{2}h = 2 + 1\frac{f(0,2) + f(1,5)}{2} = 2 + \frac{3 + 4e^{(0.8)1} - 0.5(5)}{2}1 = 6.701082. \quad (\varepsilon_t = -8.18\%)$$

True percent relative error, $\varepsilon_t = \frac{true\,value - approx}{true\,value} \cdot 100\%$

(2 iteration) corrector ($y_1^0 \leftarrow y_1$) →

$$y_1 = 2 + 1\frac{f(0,2) + f(1,6.701082)}{2} = 2 + \frac{3 + 4e^{(0.8)1} - 0.5(6.701082)}{2}1 = 6.275811. \ (\varepsilon_t = -1.31\%)$$

(3 iteration) corrector ($y_1^0 \leftarrow y_1$) →

$$y_1 = 2 + 1\frac{f(0,2) + f(1,6.275811)}{2} = 2 + \frac{3 + 4e^{(0.8)1} - 0.5(6.275811)}{2}1 = 6.382129. \quad (\varepsilon_t = -3.03\%)$$

$$y_1^1 = y_0 + \frac{f(x_0, y_0) + f(x_1, y_1^0)}{2}h$$

Repeat the iteration

Normally, we use 3 or 4 D.P. in calculation!

Ordinary differential equations (ODEs)

First-order initial value problems : **single step methods**

Improved Euler method – Heun's method

		Iterations of Heun's method			
		Iteration =1		Iteration = 15	
x	y_{true}	y_{approx}	$\lvert\varepsilon_t\rvert$ (%)	y_{approx}	$\lvert\varepsilon_t\rvert$ (%)
0	2	2	0	2	0
1	6.1946314	6.7010819	8.18	6.3608655	2.68
2	14.8439219	16.3197819	9.94	15.3022367	3.09
3	33.6771718	37.1992489	10.46	34.7432761	3.17
4	75.3389626	83.3377674	10.62	77.7350962	3.18

Normally, we use
3 or 4 D.P. in calculation!

$$\frac{dy}{dx} = f(x) \rightarrow \int_{y_i}^{y_{i+1}} dy = \int_{x_i}^{x_{i+1}} f(x)dx$$

$$\rightarrow y_{i+1} - y_i = \int_{x_i}^{x_{i+1}} f(x)dx \rightarrow \quad y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} f(x)dx$$

Trapezoidal rule for integration

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{f(x_i) + f(x_{i+1})}{2}h - \frac{h^3}{12}f''(\xi), \quad x_i < \xi < x_{i+1}.$$

$$\rightarrow y_{i+1} = y_i + \frac{f(x_i) + f(x_{i+1})}{2}h + O(h^3)$$

Local error

Heun's method is second order since second derivative of ODE is zero. Local error is $O(h^3)$.
Propagated truncated error results from the approximations produced in previous steps. The sum of two is Global truncation error.

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

Initial value problem (IVP) for a single first order DE

$y' = f(x,y)$, $y(a) = \eta$ (1)
for $a \le x \le b$.

Let
$x_n = a + nh$, $n = 0,1,2,\ldots$
h = steplength.
y_n is approximation for $y(x_n)$
$f_n \equiv f(x_n, y_n)$

Linear multistep method of stepnumber *k*, or linear *k*-step method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad (2)$$

where α_j and β_j are constants, $\alpha_k \neq 0$, not both α_0 and β_0 are zero. And let $\boldsymbol{\alpha_k = 1}$

Eq (2) is explicit if $\beta_k = 0$, implicit if $\beta_k \neq 0$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

$y' = f(x,y)$

Derivation through Taylor expansions

$$y(x+h) = y(x) + h\frac{y'(x)}{1!} + h^2\frac{y''(x)}{2!} + h^3\frac{y'''(x)}{3!} + \cdots + h^n\frac{y^{(n)}(x)}{n!} + R_n^*.$$

$$y(x-h) = y(x) - h\frac{y'(x)}{1!} + h^2\frac{y''(x)}{2!} - h^3\frac{y'''(x)}{3!} + \cdots$$

We get $y(x_n+h) - y(x_n-h) = 2hy'(x_n) + h^3\frac{2y'''(x_n)}{3!} + \cdots$

$y_{n+1} - y_{n-1} = 2hf_n + O(h^3)$ Mid-point rule $y_{n+2} - y_n = 2hf_{n+1} + O(h^3)$

Let linear multistep method in the form $y_{n+1} + \alpha_0 y_n = h(\beta_1 f_{n+1} + \beta_0 f_n)$

$$y(x_n+h) + \alpha_0 y(x_n) \cong h\left[\beta_1 y^{(1)}(x_n+h) + \beta_0 y^{(1)}(x_n)\right] \quad \text{(A)}$$

To choose α_0, β_1, β_0, we use $y(x_n+h) = y(x_n) + h\frac{y^{(1)}(x_n)}{1!} + h^2\frac{y^{(2)}(x_n)}{2!} + h^3\frac{y^{(3)}(x_n)}{3!} + \cdots$

$$y^{(1)}(x_n+h) = y^{(1)}(x_n) + h\frac{y^{(2)}(x_n)}{1!} + h^2\frac{y^{(3)}(x_n)}{2!} + h^3\frac{y^{(4)}(x_n)}{3!} + \cdots$$

Substitute in (A), we get

$$\left[y(x_n) + h\frac{y^{(1)}(x_n)}{1!} + h^2\frac{y^{(2)}(x_n)}{2!} + h^3\frac{y^{(3)}(x_n)}{3!}\right] + \alpha_0 y(x_n) \cong h\left[\beta_1\left(y^{(1)}(x_n) + h\frac{y^{(2)}(x_n)}{1!} + h^2\frac{y^{(3)}(x_n)}{2!} + h^3\frac{y^{(4)}(x_n)}{3!}\right) + \beta_0 y^{(1)}(x_n)\right]$$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

$y' = f(x,y)$

Derivation through Taylor expansions

$$y(x_n+h)+\alpha_0 y(x_n) \cong h\left[\beta_1 y^{(1)}(x_n+h)+\beta_0 y^{(1)}(x_n)\right] \qquad \text{(A)}$$

$$\left[y(x_n)+h\frac{y^{(1)}(x_n)}{1!}+h^2\frac{y^{(2)}(x_n)}{2!}+h^3\frac{y^{(3)}(x_n)}{3!}\right]+\alpha_0 y(x_n) \cong h\left[\beta_1\left(y^{(1)}(x_n)+h\frac{y^{(2)}(x_n)}{1!}+h^2\frac{y^{(3)}(x_n)}{2!}+h^3\frac{y^{(4)}(x_n)}{3!}\right)+\beta_0 y^{(1)}(x_n)\right]$$

$$(1+\alpha_0)y(x_n)+(1-\beta_1-\beta_0)hy^{(1)}(x_n)+\left(\frac{1}{2}-\beta_1\right)h^2 y^{(2)}(x_n)+\left(\frac{1}{6}-\frac{1}{2}\beta_1\right)h^3 y^{(3)}(x_n)+\cdots \cong 0$$

⇒ $C_0 y(x_n)+C_1 hy^{(1)}(x_n)+C_2 h^2 y^{(2)}(x_n)+C_3 h^3 y^{(3)}(x_n)+\cdots \cong 0$

where $C_0=1+\alpha_0$, $C_1=1-\beta_1-\beta_0$, $C_2=½-\beta_1$, $C_3=1/6\ -½\,\beta_1$

Now set $C_0=0$, $C_1=0$ & $C_2=0 \rightarrow \alpha_0=-1$, $\beta_1=\beta_0=½ \ \rightarrow C_3=-1/12$.

⇒ $y_{n+1}-y_n=\frac{h}{2}\left(f_{n+1}+f_n\right)+O\left(h^3\right)$ Trapezoidal rule

order *p* if, $C_0=C_1=\ldots=C_p=0$, $C_{p+1}\neq 0$.

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

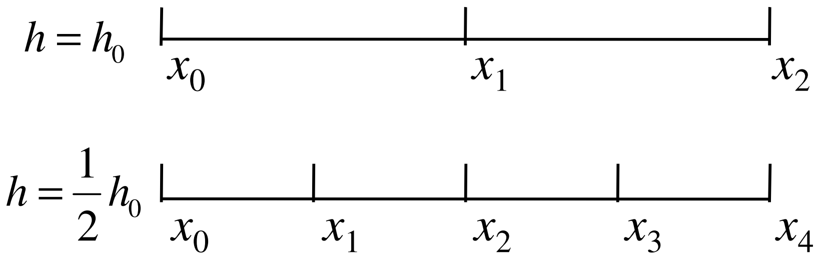
Convergence

$$y' = f(x,y),\ y(a) = \eta, \text{ for } a \le x \le b. \qquad (1)$$

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad (2)$$

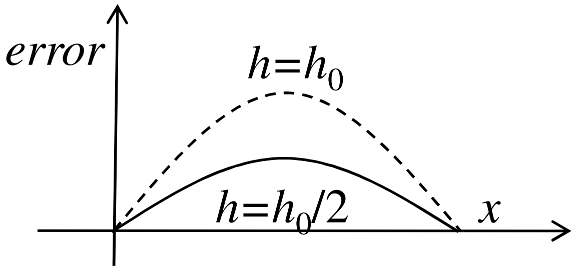
Linear *k*-step method eq(2) is **convergent** if IVP (1), subject Lipschitz condition, we have

$$\lim_{\substack{h \to 0 \\ nh = x - a}} y_n = y(x_n)$$



Given initial value problem (IVP)
$y' = f(x,y)$, $y(a) = \eta$ (1)

Lipschitz condition:
$|f(x,y) - f(x,y^*)| \le L|y - y^*|$
where L is Lipschitz costant



Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

Order and error constant

For linear mutistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad (2)$$

Let linear difference operator

$$\ell[y(x);h] = \sum_{j=0}^{k} \left[\alpha_j y(x+jh) - h\beta_j y'(x+jh)\right] \qquad (A)$$

Using Taylor series, we get

$$\ell[y(x);h] = C_0 y(x) + C_1 h y^{(1)}(x) + C_2 h^2 y^{(2)}(x) + \cdots + C_p h^p y^{(p)}(x) + \cdots = 0 \qquad (B)$$

Definition: The difference operator (A) and the associated linear multistep method (2) Are said to be of **order *p*** if, in (A), $C_0=C_1=\ldots=C_p=0$, $C_{p+1}\neq 0$.

use

$$y(x+h) = y(x) + h\frac{y'(x)}{1!} + h^2\frac{y''(x)}{2!} + h^3\frac{y'''(x)}{3!} + \cdots$$

Comparing Eq (A) and (B), we get

$$C_0 = \alpha_0 + \alpha_1 + \alpha_2 + \cdots + \alpha_k,$$

$$C_1 = \alpha_1 + 2\alpha_2 + \cdots + k\alpha_k - (\beta_0 + \beta_1 + \beta_2 + \cdots + \beta_k),$$

$$C_q = \frac{1}{q!}\left(\alpha_1 + 2^q\alpha_2 + \cdots + k^q\alpha_k\right) - \frac{1}{(q-1)!}\left(\beta_1 + 2^{q-1}\beta_2 + \cdots + k^{q-1}\beta_k\right), \; q = 2,3,\cdots$$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

Order and error constant

Example 1: Construct an implicit linear two-step method of maximal order, containing one free parameter, and find its order.

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\sum_{j=0}^{k}\beta_j f_{n+j}$$ ⇒ k=2 (step), α_2=+1

Remain 4 undetermined coefficients α_1, β_0, β_1, and β_2. ⇒ Set C_0=C_1=C_2=C_3=0

$$\left.\begin{aligned} C_0 &= a+\alpha_1+1=0,\\ C_1 &= \alpha_1+2-(\beta_0+\beta_1+\beta_2)=0,\\ C_2 &= \frac{1}{2!}(\alpha_1+4)-(\beta_1+2\beta_2)=0,\\ C_3 &= \frac{1}{3!}(\alpha_1+8)-\frac{1}{2!}(\beta_1+4\beta_2)=0. \end{aligned}\right\}$$

Solved using Linear system

$$\alpha_1=-1-a,\ \beta_0=-\frac{1}{12}(1+5a),$$

$$\beta_1=\frac{2}{3}(1-a),\ \beta_2=\frac{1}{12}(5+a).$$

Implicit linear two-step method is $$y_{n+2}-(1+a)y_{n+1}+ay_n=\frac{h}{12}\left[(5+a)f_{n+2}+8(1-a)f_{n+1}-(1+5a)f_n\right] \qquad \text{(a)}$$

Moreover,

$$C_4=\frac{1}{4!}(\alpha_1+16)-\frac{1}{3!}(\beta_1+8\beta_2)=-\frac{1}{4!}(1+a),$$

$$C_5=\frac{1}{5!}(\alpha_1+32)-\frac{1}{4!}(\beta_1+16\beta_2)=-\frac{1}{3\cdot 5!}(17+13a).$$

$$C_0=\alpha_0+\alpha_1+\alpha_2+\cdots+\alpha_k,$$

$$C_q=\frac{1}{q!}\left(\alpha_1+2^q\alpha_2+\cdots+k^q\alpha_k\right)-\frac{1}{(q-1)!}\left(\beta_1+2^{q-1}\beta_2+\cdots+k^{q-1}\beta_k\right),$$

$$q=2,3,\cdots$$

If $a\neq-1$, then $C_4\neq 0$, method (a) is of order 3.

If $a=-1$, then $C_4=0$, $C_5\neq 0$, and method (a), which is now Simpson's rule, is of order 4.

$$\ell[y(x);h]=C_0y(x)+C_1hy^{(1)}(x)+C_2h^2y^{(2)}(x)+\cdots+C_ph^py^{(p)}(x)+\cdots=0$$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

$y' = f(x,y)$

Consistency

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \qquad \text{(a)}$$

Definition: the linear multistep method (a) is **consistent** if it has order $p \geq 1$.

of **order *p*** if, in (a), $C_0 = C_1 = \ldots = C_p = 0$, $C_{p+1} \neq 0$.

$$C_0 = \alpha_0 + \alpha_1 + \alpha_2 + \cdots + \alpha_k,$$
$$C_1 = \alpha_1 + 2\alpha_2 + \cdots + k\alpha_k - (\beta_0 + \beta_1 + \beta_2 + \cdots + \beta_k),$$
$$C_q = \frac{1}{q!}\left(\alpha_1 + 2^q \alpha_2 + \cdots + k^q \alpha_k\right) - \frac{1}{(q-1)!}\left(\beta_1 + 2^{q-1}\beta_2 + \cdots + k^{q-1}\beta_k\right), \; q = 2,3,\cdots$$

$$\sum_{j=0}^{k} \alpha_j = 0 \quad ; \quad \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j \qquad \text{(b)}$$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

$y' = f(x,y)$, $y(a) = \eta$, for $a \le x \le b$.

Adams-Bashforth – open formulas

$f_i = f(x_i, y_i)$

Taylor series expansion around x_i

$$y_{i+1} = y_i + f_i h + \frac{f_i'}{2} h^2 + \frac{f_i''}{3!} h^3 + \cdots = y_i + h\left(f_i + \frac{f_i'}{2} h + \frac{f_i''}{3!} h^2 + \cdots \right)$$

Backward difference to approximate derivative: $f_i' = \frac{f_i - f_{i-1}}{h} + \frac{f_i''}{2} h + O\left(h^2\right)$

$$y_{i+1} = y_i + h\left\{ f_i + \frac{h}{2}\left[\frac{f_i - f_{i-1}}{h} + \frac{f_i''}{2} h + O\left(h^2\right) \right] + \frac{h^2}{6} f_i'' + \cdots \right\} \xrightarrow{\text{simplify}} y_{i+1} = y_i + h\left(\frac{3}{2} f_i - \frac{1}{2} f_{i-1} \right) + \frac{5}{12} h^3 f_i'' + O\left(h^4\right)$$

$$\boxed{y_{i+1} = y_i + h\left(\frac{3}{2} f_i - \frac{1}{2} f_{i-1} \right)} + O(h^3), \quad \text{2-step method.}$$

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

Coefficients and truncation error for *n*-order (open) Adams-Bashforth predictors

$$y_{i+1} = y_i + h\sum_{k=0}^{n-1} b_k f_{i-k} + O\left(h^{n+1}\right) \qquad f_i = f(x_i, y_i)$$

order	b_0	b_1	b_2	b_3	b_4	**Local truncation error**
1	1					$\frac{1}{2} h^2 f'(\xi)$
2	3/2	-1/2				$\frac{5}{12} h^3 f''(\xi)$
3	23/12	-16/12	5/12			$\frac{9}{24} h^4 f^{(3)}(\xi)$
4	55/24	-59/24	37/24	-9/24		$\frac{251}{720} h^5 f^{(4)}(\xi)$
5	1901/720	-2774/720	2616/720	-1274/720	251/720	$\frac{475}{1440} h^6 f^{(5)}(\xi)$

Adams-Moulton – closed formulas

Backward Taylor series expansion around x_{i+1}

$$y_i = y_{i+1} - f_{i+1} h + \frac{f'_{i+1}}{2} h^2 - \frac{f''_{i+1}}{3!} h^3 + \cdots \quad \rightarrow \quad y_{i+1} = y_i + h\left(f_{i+1} - \frac{h}{2} f'_{i+1} + \frac{h^2}{6} f''_{i+1} + \cdots \right)$$

Approximate 1st derivative $f'_{i+1} = \frac{f_{i+1} - f_i}{h} + \frac{f''_{i+1}}{2} h + O\left(h^2\right)$

$$\boxed{y_{i+1} = y_i + h\left(\frac{1}{2} f_{i+1} + \frac{1}{2} f_i\right) - \frac{1}{12} h^3 f''_{i+1} - O\left(h^4\right)}$$

$$y_{i+1} = y\left(x_i + h\right) = y_i + h y'_i + \frac{h^2}{2!} y''_i + \cdots$$

$$y_i = y\left(x_{i+1} - h\right) - h y'_i + \frac{h^2}{2!} y''_i - \cdots$$

Second order Adams-Moulton formula

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

Coefficients and truncation error for *n*-order (closed) Adams-Moulton correctors

$$y_{i+1} = y_i + h\sum_{k=0}^{n-1} b_k f_{i+1-k} + O\left(h^{n+1}\right)$$

$f_i = f(x_i, y_i)$

order	b_0	b_1	b_2	b_3	b_4	**Local truncation error**
2	½	½				$-\frac{1}{12}h^3 f''(\xi)$
3	5/12	8/12	-1/12			$-\frac{1}{24}h^4 f^{(3)}(\xi)$
4	9/24	19/24	-5/24	1/24		$-\frac{19}{720}h^5 f^{(4)}(\xi)$
5	251/720	646/720	-264/720	106/720	-19/720	$-\frac{27}{1440}h^6 f^{(5)}(\xi)$

y_{i+1}^{j} ← iteration

↖ node

Fourth-order Adams method (requires **4** previous values)

Predictor: $y_{i+1}^0 = y_i^m + h\left(\frac{55}{24}f_i^m - \frac{59}{24}f_{i-1}^m + \frac{37}{24}f_{i-2}^m - \frac{9}{24}f_{i-3}^m\right)$ $\Longrightarrow$ Predictor can be used alone!

Corrector: $y_{i+1}^j = y_i^m + h\left(\frac{9}{24}f_{i+1}^{j-1} + \frac{19}{24}f_i^m - \frac{5}{24}f_{i-1}^m + \frac{1}{24}f_{i-2}^m\right)$

where *j*=iteration=1,2,…,*m*.

Iterations terminate on **approximate percent relative error**, ε_a.

$$\left|\varepsilon_a\right| = \left|\frac{y_{i+1}^j - y_{i+1}^{j-1}}{y_{i+1}^j}\right| \cdot 100\%$$

Predictor calculate for y_1^0 (use y_0 and others); get y_2^0 (use y_1^m and others); …

Corrector calculate for y_1^1, y_1^2,…, y_1^m. (*m* iteration); get y_2^1, y_2^2,…, y_2^m. (*m* iteration); …

Ordinary differential equations (ODEs)

First-order initial value problems : **multistep methods**

E.g. $\boldsymbol{y'=4e^{0.8x}-0.5y}$, $0\leq x\leq 4$, step size (h=1), initial condition, $y(0)$=2.

Analytical solution: $y=(4/1.3)[e^{0.8x}-e^{-0.5x}]+2e^{-0.5x}$.

here we use analytical solution to compute exact values at

x_{-3}= -3, x_{-2}= -2, x_{-1}= -1, with y_{-3}= -4.547302, y_{-2}= -2.306160 & y_{-1}= -0.3929953.

Previous values can be approximated by Runge-Kutta method or others.

$$y'_0 = f(x_0, y_0) = f_0 = f_0^m = f(0,2) = 3,\ y'_{-1} = f(x_{-1}, y_{-1}) = f_{-1}^m = f(-1,-0.3929953) = 1.993814.$$

$$y'_{-2} = f(x_{-2}, y_{-2}) = f_{-2}^m = f(-2,-2.30616) = 1.960667,\ y'_{-3} = f(x_{-3}, y_{-3}) = f_{-3}^m = f(-3,-4.547302) = 2.6365228.$$

By setting <u>number of iterations, m=1</u>, we get

Predictor:

$$y_1^0 = y_0^m + h\left(\frac{55}{24}f_0^m - \frac{59}{24}f_{-1}^m + \frac{37}{24}f_{-2}^m - \frac{9}{24}f_{-3}^m\right)$$

$$= 2 + 1\left(\frac{55}{24}3 - \frac{59}{24}1.993814 + \frac{37}{24}1.960667 - \frac{9}{24}2.6365228\right) = 6.007539.$$

True percent relative error, $\varepsilon_t = {}^{\text{(true value-approx)}}/_{\text{(true value)}} \times 100\% = 3.1\%$

Corrector:

$$y_{i+1}^j = y_i^m + h\left(\frac{9}{24}f_{i+1}^{j-1} + \frac{19}{24}f_i^m - \frac{5}{24}f_{i-1}^m + \frac{1}{24}f_{i-2}^m\right)$$

$$f_i^m = f\left(x_i, y_i^m\right)$$

$$f_1^0 = f(x_1, y_1^0) = f(1,6.007539) = 5.898394.$$

$$y_1^1 = y_0^m + h\left(\frac{9}{24}f_1^0 + \frac{19}{24}f_0^m - \frac{5}{24}f_{-1}^m + \frac{1}{24}f_{-2}^m\right)$$

$$= 2 + 1\left(\frac{9}{24}5.898394 + \frac{19}{24}3 - \frac{5}{24}1.993814 + \frac{1}{24}1.960667\right) = 6.253214.$$

ε_t = -0.96% ⇨ improvement

Ordinary differential equations (ODEs)

First-order initial value problems : **fourth-order Runge-Kutta method (RK4)**

General formula of RK4:

$y(x+h)-y(x)\approx ak_1+bk_2+ck_3+dk_4+O(h^5)$

$k_1=hf(x,y)$, $k_2=hf(x+mh,y+mk_1)$, $k_3=hf(x+nh,y+nk_2)$, $k_4=hf(x+ph,y+pk_3)$

Note: it is fourth-order because it reproduces the terms in the Taylor series up to and include term involve h^4.

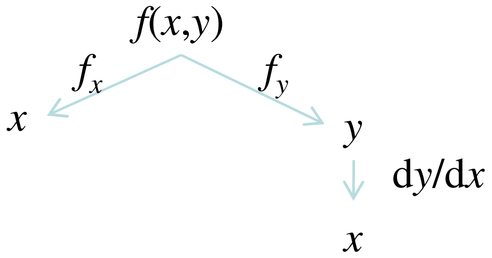
Let $F_1 = f_x + ff_y$, $F_2 = f_{xx} + 2ff_{xy} + f^2 f_{yy}$, $F_3 = f_{xxx} + 3ff_{xxy} + 3f^2 f_{xyy} + f^3 f_{yyy}$

Differentiating $y'=f(x,y)$, we find

$$y^{(2)} = \frac{d^2y}{dx^2} = f_x + f_y y' = f_x + f_y f = F_1$$

$$y^{(3)} = f_{xx} + 2ff_{xy} + f^2 f_{yy} + f_y\left(f_x + ff_y\right) = F_2 + f_y F_1$$

$$y^{(4)} = \cdots = F_3 + f_y F_2 + 3F_1\left(f_{xy} + ff_{yy}\right) + f_y^2 F_1$$



Taylor series can be written

$$y(x+h) - y(x) = hy' + \frac{1}{2!}h^2 y^{(2)} + \frac{1}{3!}h^3 y^{(3)} + \frac{1}{4!}h^4 y^{(4)} + \cdots$$

$$= hf + \frac{1}{2}h^2 F_1 + \frac{1}{6}h^3\left(F_2 + f_y F_1\right) + \frac{1}{24}h^4\left(F_3 + f_y F_2 + 3\left(f_{xy} + ff_{yy}\right)F_1 + f_y^2 F_1\right) + \cdots$$

Now, expand k_i in Taylor series:

$$k_1 = hf$$

$$k_2 = h\left[f + mhF_1 + \tfrac{1}{2}m^2h^2F_2 + \tfrac{1}{6}m^3h^3F_3 + \cdots\right]$$

$$k_3 = h\left[f + nhF_1 + \tfrac{1}{2}h^2\left(n^2F_2 + 2mnf_yF_1\right) + \cdots\right]$$

$$k_4 = h\left[f + phF_1 + \tfrac{1}{2}h^2\left(p^2F_2 + 2npf_yF_1\right) + \cdots\right]$$

Combining with $y(x+h)-y(x)\approx ak_1+bk_2+ck_3+dk_4$, we get

$$y(x+h)-y(x)=(a+b+c+d)hf+(bm+cn+dp)h^2F_1+½(bm^2+cn^2+dp^2)h^3F_2+\ldots$$

Ordinary differential equations (ODEs)

First-order initial value problems : **fourth-order Runge-Kutta method (RK4)**

Comparison with Taylor series shows that

$a+b+c+d=1$; $cmn+dnp=1/6$; $bm+cn+dp=1/2$; $cmn^2+dnp^2=1/8$

$bm^2+cn^2+dp^2=1/3$; $cm^2\mathrm{n}+dn^2p=1/12$; $bm^3+cn^3+dp^3=1/4$; $dmnp=1/24$.

8 equations with 7 unknowns. The classical solution set is: $m=n=1/2$, $p=1$, $a=d=1/6$, $b=c=1/3$.

RK4 is given

$$y(x+h)\approx y(x) +1/6[\ k_1+2k_2+2k_3+k_4]$$

$$k_1=hf(x,y),\ k_2=hf(x+ ½h,y+ ½\ k_1),\ k_3=hf(x+ ½\ h,y+ ½\ k_2),\ k_4=hf(x+h,y+k_3)$$

Note: calculation of higher derivatives of $y(x)$ is not required.

Second-order Runge-Kutta (RK2) method also called Heun's method.

$$y(x+h)\approx y(x)+ ½[\ k_1+k_2]+O(h^3)$$

$$k_1=hf(x,y),\ k_2=hf(x+h,y+k_1)$$

e.g. $y'=f(x,y)=-2x^3+12x^2-20x+8.5$, with step size $h=0.5$ and initial condition $y(0)=1$,

Find $y(-0.5)$ using RK2 and RK4. exact answer: $y(x)=-\ ½\ x^4+4x^3-10x^2+8.5x+1$.$y(-0.5)=-6.28125$.

RK2: $k_1=hf(0,1)=(-0.5)[-2(0)^3+12(0)^2-20(0)+8.5]=-4.25$, (here, $\boldsymbol{h=-0.5}$)

$k_2=hf(0-0.5,1-4.25)= (-0.5)[-2(-0.5)^3+12(-0.5)^2-20(-.5)+8.5]=-10.875$.

Answer: $y(-0.5)=y(0)+ ½[\ k_1+k_2]=1+½\ [-4.25-10.875]=-6.5625$. $\varepsilon_t=-4.5\%$.

Ordinary differential equations (ODEs)

First-order initial value problems : **fourth-order Runge-Kutta method (RK4)**

RK4: $k_1=hf(0,1)=(-0.5)[-2(0)3+12(0)2-20(0)+8.5]=-4.25$, (here, $\boldsymbol{h}$**=-0.5**)

$k_2=hf(0-0.5/2,1-4.25/2)= (-0.5)[-2(-0.25)3+12(-0.25)2-20(-.25)+8.5]=-7.140625$,

$k_3=hf(0-0.5/2,1-7.140625/2)= (-0.5)[-2(-0.25)3+12(-0.25)2-20(-.25)+8.5]=-7.140625$,

$k_4=hf(0-0.5,1-7.140625)= (-0.5)[-2(-0.5)3+12(-0.5)2-20(-.5)+8.5]= -10.875$.

Answer: $y(-0.5)=y(0)+ 1/6[k_1+2k_2+2k_3+k_4]=1+1/6 [-43.6875]=-6.28125.\rightarrow$ $\boldsymbol{\varepsilon_t=0\%}$.

Note: RK4 produce exact solution since true solution is a quartic. The fourth-order method gives an exact result.

E.g. $\boldsymbol{y'=4e^{0.8x}-0.5y}$, $0\leq x\leq 0.5$, step size (h=0.5), initial condition, $y(0)=2$.

Analytical solution: $y=(4/1.3)[e^{0.8x}-e^{-0.5x}]+2e^{-0.5x}$. $y(0.5)=3.751521$

RK4: $k_1=hf(0,2)=(0.5)[4e^{0.8(0)}-0.5(2)]=1.5$, (here, $\boldsymbol{h}$**=0.5**)

$k_2=hf(0+0.5/2,2+1.5/2)=(0.5)[4e^{0.8(0.25)}-0.5(2.75)]=1.755306$,

$k_3=hf(0+0.5/2,2+1.755306/2)= (0.5)[4e^{0.8(0.25)}-0.5(2.877653)]=1.723392$,

$k_4=hf(0+0.5,2+1.723392)= (0.5)[4e^{0.8(0.5)}-0.5(3.723392)]=2.052801$,

Answer: $y(0.5)=y(0)+ 1/6[k1+2k2+2k3+k4]=2+1/6 [-43.6875]=3.7516995 \rightarrow$ $\boldsymbol{\varepsilon_t=-0.0048\%}$.

Ordinary differential equations (ODEs)

Systems of first-order initial value problems

Standard form for a system of first-order ODEs is:

$$
\begin{aligned}
x_1' &= f_1(t, x_1, x_2, \cdots, x_n) \\
x_2' &= f_2(t, x_1, x_2, \cdots, x_n) \\
&\vdots \\
x_n' &= f_n(t, x_1, x_2, \cdots, x_n)
\end{aligned}
$$

$$x_1' = \frac{d}{dt} x_1$$

Example of system of first-order ODEs is given:

$$\boldsymbol{x' = x + 4y - e^t} \quad , \quad \boldsymbol{y' = x + y + 2e^t}.$$

The general solution is

$$\boldsymbol{x = 2ae^{3t} - 2be^{-t} - 2e^t} \quad , \quad \boldsymbol{y = ae^{3t} + be^{-t} + 1/4\ e^t},$$

where a and b are arbitrary constants.

If the system were given initial conditions

$x(0)=4, \quad y(0)=5/4,$

Then the particular solution would be

$$\boldsymbol{x = 4e^{3t} + 2e^{-t} - 2e^t} \quad , \quad \boldsymbol{y = 2e^{3t} - e^{-t} + 1/4\ e^t}.$$

Ordinary differential equations (ODEs)

Systems of first-order initial value problems

Let X denote column vector whose components are $x_1, x_2, \ldots, x_n$. These components are functions of t. And let F denote column vector with components $f_1, f_2, \ldots, f_n$.

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, F = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix} \quad \text{system of ODE} \rightarrow X' = F(t, X) \Leftrightarrow \begin{bmatrix} \frac{d}{dt} x_1 \\ \frac{d}{dt} x_2 \\ \vdots \\ \frac{d}{dt} x_n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}.$$

e.g. convert the initial-value problem

$(\sin t)y''' + \cos(ty) + \sin(t^2 + y'') + (y')^3 = \ln t$

$y(2)=7, \quad y'(2)=3, \quad y''(2)=-4,$

into a system of ODEs.

Solution: introduce new variables x_1,x_2 & x_3 as: $x_1=y$, $x_2=y'$, and $x_3=y''$. The system of ODEs for $X=[x_1, x_2, x_3]^T$ is

$x_1'=x_2, \quad x_2'=x_3, \quad x_3'=[\ln t - x_2^3 - \sin(t^2+x_3) - \cos(tx_1)]/\sin t,$

with initial conditions at t=2 are $X=(7,3,-4)^T$.

$$X' = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}' = F = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ \left[\ln t - x_2^3 - \sin\left(t^2 + x_3\right) - \cos\left(tx_1\right)\right] \Big/ \sin t \end{bmatrix}$$

Ordinary differential equations (ODEs)

Systems of first-order initial value problems

e.g. convert the problem

$(x'')^2+te^y+y'=x'-x$, $y'y''-\cos(xy)+\sin(tx'y)=x$.

into a system of first order ODEs.

Solution: introduce new variables as: $x_1=x$, $x_2=x'$, $x_3=y$ and $x_4=y'$. The system of ODEs for $X=[x_1, x_2, x_3, x_4]^T$ is

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= \left(x_2 - x_1 - x_4 - te^{x_3}\right)^{1/2} \\ x_3' &= x_4 \\ x_4' &= \left[x_1 - \sin\left(tx_2x_3\right) + \cos\left(x_1x_3\right)\right]/x_4 \end{aligned}$$

$$\boxed{\begin{array}{l} X''(t) = \frac{d}{dt} F\left(t, X\right) \\ x_1(t),\ x_2(t),\cdots \end{array}}$$

Taylor series for column vector of X can be written as:

$$X(t+h) = X(t) + hX'(t) + \frac{h^2}{2!}X''(t) + \frac{h^3}{3!}X^{(3)}(t) + \cdots$$

$$X(t+h) \approx X(t) + hX'(t) + \frac{h^2}{2!}X''(t) + O(h^3) \leftarrow\text{----}$$ Second-order Taylor series method

$$X(t+h) \approx X(t) + hX'(t) + O(h^2) \leftarrow\text{-------------}$$ First-order Taylor series method

First-order Taylor series or Euler method for system of ODEs, $X'=F(t,X)$ is

$$\boldsymbol{X(t+h)=X(t)+hF(t,X)}$$

Ordinary differential equations (ODEs)

Systems of first-order initial value problems

Optimal RK2 method

$$X_{i+1} \approx X_i + \frac{1}{4}\left(K_1 + 3K_2\right)$$

$$K_1 = hF\left(t, X_i\right)$$

$$K_2 = hF\left(t + \frac{2}{3}h, X_i + \frac{2}{3}K_1\right)$$

, i=0, 1 2, …

Example of system of first-order ODEs is given:

$$\boldsymbol{x' = x + 4y - e^t} \qquad , \qquad \boldsymbol{y' = x + y + 2e^t.}$$

with initial conditions, $x(0)=4$, $y(0)=5/4$. Calculate $x(0.2)$ and $y(0.2)$ with Euler method.

The particular solution is given $\boldsymbol{x=4e^{3t}+2e^{-t}-2e^t}$, $\boldsymbol{y=2e^{3t}-e^{-t}+1/4\ e^t}$**.** $x(0.2)=6.483131$, $y(0.2)=3.130858$.

Here, h=0.2.

$$X(0+h) = X(0.2) = X(0) + hF(t=0)$$

$$\begin{bmatrix} x_{0.2} \\ y_{0.2} \end{bmatrix} \approx \begin{bmatrix} x(0) \\ y(0) \end{bmatrix} + 0.2\begin{bmatrix} 4+4(5/4)-e^0 \\ 4+5/4+2e^0 \end{bmatrix} = \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + 0.2\begin{bmatrix} 8 \\ 7.25 \end{bmatrix} = \begin{bmatrix} 5.6 \\ 2.7 \end{bmatrix}.$$

$$F' = {}^{d}\!/_{dt}\, F = \frac{d}{dt}\begin{bmatrix} x+4y-e^t \\ x+y+2e^t \end{bmatrix}$$

$$= \begin{bmatrix} x'+4y'-e^t \\ x'+y'+2e^t \end{bmatrix} = \begin{bmatrix} 5x+8y+6e^t \\ 2x+5y+3e^t \end{bmatrix}$$

The error vector, E is given as:

E=trues value-approximate values=[6.483131, 3.130858]-[5.6, 2.7]=[0.883131, 0.430858]

The size of error vector can be measured using different norms as below:

Euclidean norm: -----------→ $\left\|E\right\|_e = \sqrt{\sum_{i=1}^{n} e_i^2} = \sqrt{0.883131^2 + 0.430858^2} = 0.9826$

p-norm: ---------------------→ $\left\|E\right\|_p = \left(\sum_{i=1}^{n} \left|e_i\right|^p\right)^{1/p} = \left(\left|0.883131\right|^p + \left|0.430858\right|^p\right)^{1/p}$

1-norm: ---------------------→ $\left\|E\right\|_1 = \sum_{i=1}^{n} \left|e_i\right| = \left|0.883131\right| + \left|0.430858\right| = 1.313989$

Maximum-magnitude -----→ $\left\|E\right\|_\infty = \max_{1 \le i \le n} \left|e_i\right| = \max\left(\left|0.883131\right|, \left|0.430858\right|\right) = 0.883131$
or *uniform-vector* norm:

$X_0 \quad \rightarrow \quad X_{0.1} \quad \rightarrow \quad X_{0.2}$
Error: $O(0.1^2)$ $O(0.1^2)$ Σerror=const×0.02

$X_0 \quad \rightarrow \quad X_{0.2}$
Error: $O(0.2^2)$ Σerror=const×0.04

Ordinary differential equations (ODEs)

Systems of first-order initial value problems

Let X denote column vector whose components are $x_1, x_2, \ldots, x_n$. These components are functions of t.
And let F denote column vector with components $f_1, f_2, \ldots, f_n$.
The classical fourth-order Runge-Kutta (RK4), in vector form, for system of ODE are:

$$X(t+h)=X(t)+1/6(F_1+2F_2+2F_3+F_4)+O(h^5)$$

where

$$F_1=hF(t,X),\ F_2=hF(t+½h,X+½F_1),\ F_3=hF(t+½h,X+½F_2),\ F_4=hF(t+h,X+F_3).$$

$$X' = F(t,X) = \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

Previous e.g. : $\boldsymbol{x'=x+4y-e^t}$**,** $\boldsymbol{y'=x+y+2e^t}$**.**

with initial conditions, $x(0)=4$, $y(0)=5/4$. Calculate $x(0.2)$ and $y(0.2)$ with RK4.

The particular solution is given $\boldsymbol{x=4e^{3t}+2e^{-t}-2e^t}$, $\boldsymbol{y=2e^{3t}-e^{-t}+1/4\ e^t}$**.** $x(0.2)=6.483131$, $y(0.2)=3.130858$.

Here, $h=0.2$, $t=0$.

$$X = X(t=0) = \begin{bmatrix} 4 \\ 5/4 \end{bmatrix}, \quad F(t,X) = \begin{bmatrix} 4+4(5/4)-e^0 \\ 4+5/4+2e^0 \end{bmatrix} = \begin{bmatrix} 8 \\ 7.25 \end{bmatrix}, \quad F_1 = hF(t,X) = 0.2\begin{bmatrix} 8 \\ 7.25 \end{bmatrix} = \begin{bmatrix} 1.6 \\ 1.45 \end{bmatrix}.$$

$$F_2 = hF(t+½h, X+½F_1) = 0.2F\left(0.1, \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + ½\begin{bmatrix} 1.6 \\ 1.45 \end{bmatrix}\right) = 0.2F\left(0.1, \begin{bmatrix} 4.8 \\ 1.975 \end{bmatrix}\right) = 0.2\begin{bmatrix} 4.8+4(1.975)-e^{0.1} \\ 4.8+1.975+2e^{0.1} \end{bmatrix} = \begin{bmatrix} 2.318966 \\ 1.797068 \end{bmatrix}$$

$$F_3 = hF(t+½h, X+½F_2) = 0.2F\left(0.1, \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + ½\begin{bmatrix} 2.318966 \\ 1.797068 \end{bmatrix}\right) = 0.2F\left(0.1, \begin{bmatrix} 5.159483 \\ 2.148534 \end{bmatrix}\right) = 0.2\begin{bmatrix} 5.159483+4(2.148534)-e^{0.1} \\ 5.159483+2.148534+2e^{0.1} \end{bmatrix} = \begin{bmatrix} 2.52969 \\ 1.903672 \end{bmatrix}$$

$$F_4 = hF(t+h, X+F_3) = 0.2F\left(0.2, \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + \begin{bmatrix} 2.52969 \\ 1.903672 \end{bmatrix}\right) = 0.2F\left(0.2, \begin{bmatrix} 6.52969 \\ 3.153672 \end{bmatrix}\right) = 0.2\begin{bmatrix} 6.52969+4(3.153672)-e^{0.2} \\ 6.52969+3.153672+2e^{0.2} \end{bmatrix} = \begin{bmatrix} 3.584595 \\ 2.425234 \end{bmatrix}$$

$$X(0.2) = X(0) + ⅙(F_1+2F_2+2F_3+F_4) = \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + ⅙\left(\begin{bmatrix} 1.6 \\ 1.45 \end{bmatrix} + 2\begin{bmatrix} 2.318966 \\ 1.797068 \end{bmatrix} + 2\begin{bmatrix} 2.52969 \\ 1.903672 \end{bmatrix} + \begin{bmatrix} 3.584595 \\ 2.425234 \end{bmatrix}\right) = \begin{bmatrix} 6.480318 \\ 3.129452 \end{bmatrix}.$$

Error vector, $E=[6.483131,3.130858]^T-[6.480318,3.129452]^T=[0.002813,0.001406]^T$.

Maximum-magnitude norm, $\|E\|_\infty=\max(|0.002813|,|0.001406|)=\mathbf{0.002813}$.

Ordinary differential equations (ODEs)

Finite difference method for linear second-order boundary value problem

General form: $y''+p(x)y'+q(x)y=r(x)$, $a\leq x\leq b$, $y(a)=\alpha$, $y(b)=\beta$. (a)

Centered-difference formula for second derivative:

$$y''(x_i)=\frac{1}{h^2}[y(x_{i+1})-2y(x_i)+y(x_{i-1})]-\frac{h^2}{12}y^{(4)}(\xi_i),\quad x_{i-1}<\xi_i<x_{i+1}.$$

Centered-difference formula for first derivative:

$$y'(x_i)=\frac{1}{2h}[y(x_{i+1})-y(x_{i-1})]-\frac{h^2}{6}y^{(3)}(\xi_i),\quad x_{i-1}<\xi_i<x_{i+1}.$$

Let divide the interval $[a,b]$ into N equal subintervals where $x_0=a$, $x_i=x_0+ih$, $\{i=1,2,\ldots,N\}$, $x_N=b$ and $h=(b-a)/N$.

At point $x=x_i$, equation (a) becomes

$$y_i''+p_iy_i'+q_iy_i=r_i,$$

Using centered-difference formula, we get

$$\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+p_i\frac{y_{i+1}-y_{i-1}}{2h}+q_iy_i=r_i,\ (\times h^2)\rightarrow(y_{i+1}-2y_i+y_{i-1})+p_i\frac{h}{2}(y_{i+1}-y_{i-1})+h^2q_iy_i=h^2r_i$$

$$\left(1-\frac{h}{2}p_i\right)y_{i-1}-\left(2-h^2q_i\right)y_i+\left(1+\frac{h}{2}p_i\right)y_{i+1}=h^2r_i.$$

For $i=1,2,\ldots,N$-1, the above equation will produce system (N-1) equations with unknowns $y_0,y_1,\ldots,y_N$. With the given boundary condition, $y_0=\alpha$ and $y_N=\beta$, the system can be solved for $y_1,y_2,\ldots,y_{N-1}$ in matrix form, **Ay=b** (where matrix **A** is tridiagonal matrix with diagonally dominant, $|a_{ii}|>\sum|a_{ij}|$, $j=1\ldots n$, $j\neq n$, row direction).

Tridiagonal system, **Ay=b**, can be solved using Thomas algorithm.

Ordinary differential equations (ODEs)

Finite difference method for linear second-order boundary value problem

Thomas algorithm

For tridiagonal system with size $n\times n$, **Ax=b**, matrix **A** can be factored into **A=LU**, where **L** (lower triangular Matrix) and **U**(upper triangular matrix) as below:

$$A = LU \rightarrow \begin{pmatrix} d_1 & e_1 & 0 & \cdots & 0 \\ c_2 & d_2 & e_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & c_{n-1} & d_{n-1} & e_{n-1} \\ 0 & \cdots & 0 & c_n & d_n \end{pmatrix} = \begin{pmatrix} \alpha_1 & 0 & 0 & \cdots & 0 \\ c_2 & \alpha_2 & 0 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & c_{n-1} & \alpha_{n-1} & 0 \\ 0 & \cdots & 0 & c_n & \alpha_n \end{pmatrix} \cdot \begin{pmatrix} 1 & \beta_1 & 0 & \cdots & 0 \\ 0 & 1 & \beta_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & 1 & \beta_{n-1} \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix}$$

According to the above system, α_i and β_i can be calculated as

$\alpha_1=d_1$; $\alpha_i=d_i-c_i\beta_{i-1}$, $i=2,3,\ldots,n$; $\beta_i=e_i/\alpha_i$, $i=1,2,\ldots,n-1$.

The system **Ax=b** can be factorized as **LUx=b**, by letting **w=Ux**, we get **Lw=b**, then

(1) Solve **Lw=b** by forward substitution, we get

$$w_1=b_1/\alpha_1, \qquad w_i=(b_i-c_iw_{i-1})/\alpha_i,\ i=2,3,\ldots,n.$$

(2)Solve **Ux=w** by backward substitution, we get

$$x_n=w_n, \qquad x_i=w_i-\beta_ix_{i+1},\ i=n-1,\ n-2,\ldots,1.$$

The whole Thomas algorithm can be summarized as:

1. $\alpha_1=d_1$
2. $\alpha_i=d_i-c_i\beta_{i-1}$, $i=2,3,\ldots,n$
3. $\beta_i=e_i/\alpha_i$, $i=1,2,\ldots,n-1$.
4. $w_1=b_1/\alpha_1$
5. $w_i=(b_i-c_iw_{i-1})/\alpha_i$, $i=2,3,\ldots,n$.
6. $x_n=w_n$
7. $x_i=w_i-\beta_ix_{i+1}$, $i=n-1, n-2,\ldots,1$.

Ordinary differential equations (ODEs)

Finite difference method for linear second-order boundary value problem

Solve the linear boundary value problem

$$\boldsymbol{y''+(1/x)y'-(1/x^2)y=3, \quad y(1)=2, \; y(2)=3}$$

for x=1(0.2)2 using finite difference method. Analytical solution: $y(x)=x(x\text{-}1)+2/x$.

Let h=0.2, x_0=a=1, x_1=1.2, x_2=1.4, x_3=1.6, x_4=1.8 and x_5=b=2. Find $y_i \approx y(x_i)$, i=1,2,3,4.

At x_i, we get

$$y_i''+\left(\frac{1}{x_i}\right)y_i'-\left(\frac{1}{x_i^2}\right)y_i=3 \quad\rightarrow\quad \left(\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}\right)+\left(\frac{1}{x_i}\right)\left(\frac{y_{i+1}-y_{i-1}}{2h}\right)-\left(\frac{1}{x_i^2}\right)y_i=3$$

Multiply with h^2, here we use 4 decimal place.

$$\left(y_{i+1}-2y_i+y_{i-1}\right)+\frac{h}{2}\left(\frac{1}{x_i}\right)\left(y_{i+1}-y_{i-1}\right)-h^2\left(\frac{1}{x_i^2}\right)y_i=3h^2 \quad\rightarrow\quad \left(1-\frac{0.1}{x_i}\right)y_{i-1}-\left[2+\left(\frac{0.2}{x_i}\right)^2\right]y_i+\left(1+\frac{0.1}{x_i}\right)y_{i+1}=0.12$$

For i=1, $$\left(1-\frac{0.1}{x_1}\right)y_0-\left[2+\left(\frac{0.2}{x_1}\right)^2\right]y_1+\left(1+\frac{0.1}{x_1}\right)y_2=0.12 \quad\rightarrow\quad \left(1-\frac{0.1}{1.2}\right)2-\left[2+\left(\frac{0.2}{1.2}\right)^2\right]y_1+\left(1+\frac{0.1}{1.2}\right)y_2=0.12$$

$$\rightarrow \quad -2.0278y_1+1.0833y_2=-1.7133$$

For i=2, $$\left(1-\frac{0.1}{x_2}\right)y_1-\left[2+\left(\frac{0.2}{x_2}\right)^2\right]y_2+\left(1+\frac{0.1}{x_2}\right)y_3=0.12 \quad\rightarrow\quad \left(1-\frac{0.1}{1.4}\right)y_1-\left[2+\left(\frac{0.2}{1.4}\right)^2\right]y_2+\left(1+\frac{0.1}{1.4}\right)y_3=0.12$$

$$\rightarrow \quad 0.9286y_1-2.0204y_2+1.0714y_3=0.12$$

For i=3, $$\left(1-\frac{0.1}{x_3}\right)y_2-\left[2+\left(\frac{0.2}{x_3}\right)^2\right]y_3+\left(1+\frac{0.1}{x_3}\right)y_4=0.12 \quad\rightarrow\quad \left(1-\frac{0.1}{1.6}\right)y_2-\left[2+\left(\frac{0.2}{1.6}\right)^2\right]y_3+\left(1+\frac{0.1}{1.6}\right)y_4=0.12$$

$$\rightarrow \quad 0.9375y_2-2.0156y_3+1.0625y_4=0.12$$

For i=4, $$\left(1-\frac{0.1}{x_4}\right)y_3-\left[2+\left(\frac{0.2}{x_4}\right)^2\right]y_4+\left(1+\frac{0.1}{x_4}\right)y_5=0.12 \quad\rightarrow\quad \left(1-\frac{0.1}{1.8}\right)y_3-\left[2+\left(\frac{0.2}{1.8}\right)^2\right]y_4+\left(1+\frac{0.1}{1.8}\right)(3)=0.12$$

$$\rightarrow \quad 0.9444y_3-2.0123y_4=-3.0468$$

Ordinary differential equations (ODEs)

Finite difference method for linear second-order boundary value problem

Finally, we get the tridiagonal system as below:

$$\mathbf{Ay} = \mathbf{b} \quad \rightarrow \begin{pmatrix} -2.0278 & 1.0833 & 0 & 0 \\ 0.9286 & -2.0204 & 1.0714 & 0 \\ 0 & 0.9375 & -2.0156 & 1.0625 \\ 0 & 0 & 0.9444 & -2.0123 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} -1.7133 \\ 0.1200 \\ 0.1200 \\ -3.0468 \end{pmatrix}$$

Using Thomas algorithm, we get

i	**1**	**2**	**3**	**4**
d_i e_i c_i b_i	-2.0278 - 1.0833 -1.7133	-2.0204 0.9286 1.0714 0.1200	-2.0156 0.9375 1.0625 0.1200	-2.0123 0.9444 - -3.0468
$(\alpha_1=d_1)$ $\alpha_i=d_i-c_i\beta_{i-1}$,	-2.0278	-1.5243	-1.3566	-1.2726
$\beta_i=e_i/\alpha_i$,	-0.5342	-0.7029	-0.7832	-
$(w_1=b_1/\alpha_1)$ $w_i=(b_i-c_iw_{i-1})/\alpha_i$,	0.8449	0.4360	0.2128	2.5521
$(y_n=w_n)$ $y_i=w_i-\beta_iy_{i+1}$,	1.9082	1.9905	2.2116	2.5521

Finally, we get $y(1.2)\approx y_1=1.9082$, $y_2=1.9905$, $y_3=2.2116$ and $y(1.8)\approx y_4=2.5521$.
The exact solution is given as $y(1.2)=1.9067$, $y(1.4)=1.9886$, $y(1.6)=2.2100$, $y(1.8)=2.5511$.
So, finite difference method produce results accurate up to 2 decimal places.

Ordinary differential equations (ODEs)

Finite difference method for linear second-order BVP – **artificial singularity**

Solve the linear boundary value problem

$$u'' + \frac{1}{x}u' = \left(\frac{8}{8-x^2}\right)^2, \qquad u'(0)=u(1)=0. \qquad \text{Exact solution:} \quad u(x) = 2\ln\left(\frac{7}{8-x^2}\right)$$

Let h=0.2, x_0=a=0, x_1=0.2, x_2=0.4, x_3=0.6, x_4=0.8 and x_5=b=1.

We get: $\dfrac{u_0'}{x_0} = \text{singular}$ Exact solution not singular: $u(x_0)$

For Neumann BC at x_0, we get $$\lim_{x\to 0}\frac{u'(x)}{x} \xrightarrow{L'Hopital\ rule} \lim_{x\to 0}\frac{u''(x)}{1} = u''(0).$$

So, we get $$\left(\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}\right)+\left(\frac{1}{x_i}\right)\left(\frac{u_{i+1}-u_{i-1}}{2h}\right)=\left(\frac{8}{8-x_i^2}\right)^2, i=1,2,3,4 \qquad u''(0)+u''(0)=\left(\frac{8}{8-0^2}\right)^2=1$$

Use Neumann BC, we get

$$2u_0-2u_1=-\frac{1}{2}h^2=-0.02$$

$$(u_2-2u_1+u_0)+\left(\frac{0.1}{0.2}\right)(u_2-u_0)=0.04\left(\frac{8}{8-0.2^2}\right)^2$$

$$(u_3-2u_2+u_1)+\left(\frac{0.1}{0.4}\right)(u_3-u_1)=0.04\left(\frac{8}{8-0.4^2}\right)^2$$

$$(u_4-2u_3+u_2)+\left(\frac{0.1}{0.6}\right)(u_4-u_2)=0.04\left(\frac{8}{8-0.6^2}\right)^2 \qquad (0-2u_4+u_3)+\left(\frac{0.1}{0.8}\right)(0-u_3)=0.04\left(\frac{8}{8-0.8^2}\right)^2$$

Try: $$\frac{1}{x}\frac{d}{dx}(xy')=1, \; y'(0)=0, \; y(1)=10.$$

$$y=\frac{x^2}{4}+a\ln x+b=\frac{x^2}{4}+9.75$$

Ordinary differential equations (ODEs)

Finite difference method for nonlinear second-order boundary value problem

For the general nonlinear boundary value problem

$$\boldsymbol{y''=f(x,y,y'),\qquad a\le x\le b,\ y(a)=\alpha,\ y(b)=\beta,}\qquad (a)$$

Let divide the interval $[a,b]$ into N equal subintervals where $x_0=a$, $x_i=x_0+ih$, $\{i=1,2,\ldots,N\}$, $x_N=b$ and $h=(b\text{-}a)/N$.

At point $x=x_i$, equation (a) becomes

$$-\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+f\left(x_i,y_i,\frac{y_{i+1}-y_{i-1}}{2h}\right)=0\quad\rightarrow\quad\boxed{-y_{i-1}+2y_i-y_{i+1}+h^2f\left(x_i,y_i,\frac{y_{i+1}-y_{i-1}}{2h}\right)=0=f_i\left(y_1,\cdots,y_{N-1}\right)}$$

For i=1,2,…,N-1, the above equation will produce nonlinear system (N-1) equations with unknowns $y_0,y_1,\ldots,y_N$. The above nonlinear system has a unique solution if $h<2/L$, $L=\max|f_{y'}(x,y,y')|$. With the given boundary condition, $y_0=\alpha$ and $y_N=\beta$, the system can be solved by Newton's method for nonlinear systems. A sequence of iteration will converge to solution if the guess initial approximation is sufficiently close to solution.

The Jacobian matrix, $J(y_1,\ldots,y_{N\text{-}1})$ is tridiagonal with ij-th entry:

$$J\left(y_1,\cdots,y_{N-1}\right)_{ij}=\begin{cases}-1+\dfrac{h}{2}f_{y'}\left(x_i,y_i,\dfrac{y_{i+1}-y_{i-1}}{2h}\right), & for\ i=j-1\ and\ j=2,\cdots,N-1,\\ 2+h^2f_y\left(x_i,y_i,\dfrac{y_{i+1}-y_{i-1}}{2h}\right), & for\ i=j\ and\ j=1,\cdots,N-1,\\ -1-\dfrac{h}{2}f_{y'}\left(x_i,y_i,\dfrac{y_{i+1}-y_{i-1}}{2h}\right), & for\ i=j+1\ and\ j=1,\cdots,N-2.\end{cases}$$

Correction vector can be calculated using Thomas algorithm:

$$\boxed{J\cdot\begin{bmatrix}h_1^{(k)}\\ \vdots\\ h_{N-1}^{(k)}\end{bmatrix}=-\begin{bmatrix}f_1\left(y_1,\cdots,y_{N-1}\right)\\ \vdots\\ f_{N-1}\left(y_1,\cdots,y_{N-1}\right)\end{bmatrix}\quad\rightarrow\quad\begin{bmatrix}y_1^{(k+1)}\\ \vdots\\ y_{N-1}^{(k+1)}\end{bmatrix}=\begin{bmatrix}y_1^{(k)}\\ \vdots\\ y_{N-1}^{(k)}\end{bmatrix}+\begin{bmatrix}h_1^{(k)}\\ \vdots\\ h_{N-1}^{(k)}\end{bmatrix}.}$$

The Newton iteration will stop when the solutions converge to certain decimal places or some norm stopping criteria.

Ordinary differential equations (ODEs)

Finite difference method for nonlinear second-order boundary value problem

Newton's method for nonlinear systems

$$\begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

The system of equations $g_i(y_1,y_2,\ldots,y_n)=0$ $(1 \le i \le n)$
can be expressed simply as $\mathbf{G}(\mathbf{Y})=\mathbf{0}$
by letting $\mathbf{Y}=(y_1,y_2,\ldots,y_n)^T$ and $\mathbf{G}=(g_1,g_2,\ldots,g_n)^T$. Using the Taylor's series expansion, we get

$$\mathbf{0}=\mathbf{G}(\mathbf{Y}+\mathbf{H}) \approx \mathbf{G}(\mathbf{Y})+\mathbf{G}'(\mathbf{Y})\mathbf{H} \ ,$$ *(where* $\mathbf{Y}+\mathbf{H}$ *is more accurate solution)*

where $\mathbf{H}=(h_1,h_2,\ldots,h_n)^T$ and $\mathbf{G}'(\mathbf{Y})$ is the $n \times n$ Jacobian matrix $\mathbf{J}(\mathbf{Y})$:

$$\mathbf{J}(\mathbf{Y}) = \mathbf{G}'(\mathbf{Y}) = \begin{bmatrix} \partial g_1/\partial y_1 & \partial g_1/\partial y_2 & \cdots & \partial g_1/\partial y_n \\ \partial g_2/\partial y_1 & \partial g_2/\partial y_2 & \cdots & \partial g_2/\partial y_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial g_n/\partial y_1 & \partial g_n/\partial y_2 & \cdots & \partial g_n/\partial y_n \end{bmatrix}$$

$y'' + (y')^3 y = 0$

$ans: y^3/3 - 2c_1 y = 2x + c2$

$let\, c_1 = c_2 = 0$

$y^3 = 6x$

$x = 1(0.25)2$

The correction vector $\mathbf{H}$ is obtained by solving linear system

$$\mathbf{J}(\mathbf{Y})\mathbf{H} = -\mathbf{G}(\mathbf{Y})$$

If Jacobian matrix is tridiagonal matrix, then $\mathbf{H}$ can be solved using Thomas algorithm. If the matrix size is 2×2, then just use the inverse of matrix $\mathbf{J}$, $\mathbf{H}=\mathbf{J}^{-1}(-\mathbf{G})$.
Finally, Newton's iteration for n nonlinear equations in n variables is given by

$$\mathbf{Y}^{(k+1)}=\mathbf{Y}^{(k)}+\mathbf{H}^{(k)}$$

where the Jacobian system is

$$\mathbf{J}(\mathbf{Y}^{(k)})\mathbf{H}^{(k)} = -\mathbf{G}(\mathbf{Y}^{(k)}).$$

Ordinary differential equations (ODEs)

Finite difference method for nonlinear second-order boundary value problem

E.g. use nonlinear finite difference method to solve boundary value problem

$$y'' = -(y')^2 - y + \ln x,\quad 1 \le x \le 2,\ y(1)=0,\ y(2)=\ln 2=0.6931.$$

for $x=1(0.2)2$. Analytical solution: $y=\ln x$. (use 4 decimal places). Stopping criterion: Tolerance, $\varepsilon=0.02$ using *maximum-magnitude* norm.

Let $h=0.2$, $x_0=a=1$, $x_1=1.2$, $x_2=1.4$, $x_3=1.6$, $x_4=1.8$ and $x_5=b=2$. Find $y_i \approx y(x_i)$, $i=1,2,3,4$. $N=5$.

At x_i, we get

$$-\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+f\left(x_i, y_i, \frac{y_{i+1}-y_{i-1}}{2h}\right)=0 \quad \to \boxed{-y_{i-1}+2y_i-y_{i+1}+h^2\left(-\left(\frac{y_{i+1}-y_{i-1}}{2h}\right)^2-y_i+\ln x_i\right)=0=g_i}$$

For $i=1$, $$-y_0+2y_1-y_2+0.2^2\left(-\left(\frac{y_2-y_0}{2(0.2)}\right)^2-y_1+\ln x_1\right)=0 \to -0+2y_1-y_2+\left(-\frac{1}{4}(y_2-0)^2-0.2^2y_1+0.2^2\cdot 0.1823\right)=0=g_1$$

For $i=2$, $$-y_1+2y_2-y_3+0.2^2\left(-\left(\frac{y_3-y_1}{2(0.2)}\right)^2-y_2+\ln x_2\right)=0 \to -y_1+2y_2-y_3+\left(-\frac{1}{4}(y_3-y_1)^2-0.2^2y_2+0.2^2\cdot 0.3365\right)=0=g_2$$

For $i=3$, $$-y_2+2y_3-y_4+0.2^2\left(-\left(\frac{y_4-y_2}{2(0.2)}\right)^2-y_3+\ln x_3\right)=0 \to -y_2+2y_3-y_4+\left(-\frac{1}{4}(y_4-y_2)^2-0.2^2y_3+0.2^2\cdot 0.4700\right)=0=g_3$$

For $i=4$, $$-y_3+2y_4-y_5+0.2^2\left(-\left(\frac{y_5-y_3}{2(0.2)}\right)^2-y_4+\ln x_4\right)=0 \to -y_3+2y_4-0.6931+\left(-\frac{1}{4}(0.6931-y_3)^2-0.2^2y_4+0.2^2\cdot 0.5878\right)=0=g_4$$

$$\mathbf{J}(\mathbf{Y})=\begin{bmatrix} \partial g_1/\partial y_1 & \partial g_1/\partial y_2 & \cdots & \partial g_1/\partial y_4 \\ \partial g_2/\partial y_1 & \partial g_2/\partial y_2 & \cdots & \partial g_2/\partial y_4 \\ \partial g_3/\partial y_1 & \partial g_3/\partial y_2 & \ddots & \vdots \\ \partial g_4/\partial y_1 & \partial g_4/\partial y_2 & \cdots & \partial g_4/\partial y_4 \end{bmatrix}=\begin{bmatrix} 2-0.2^2 & -1-\tfrac{1}{2}(y_2-\mathbf{0}) & 0 & 0 \\ -1-\tfrac{1}{2}(y_3-y_1)(-1) & 2-0.2^2 & -1-\tfrac{1}{2}(y_3-y_1) & 0 \\ 0 & -1-\tfrac{1}{2}(y_4-y_2)(-1) & 2-0.2^2 & -1-\tfrac{1}{2}(y_4-y_2) \\ 0 & 0 & -1-\tfrac{1}{2}(\mathbf{0.6931}-y_3)(-1) & 2-0.2^2 \end{bmatrix}$$

Ordinary differential equations (ODEs)

Finite difference method for nonlinear second-order boundary value problem

$$\mathbf{J}(\mathbf{Y})=\begin{bmatrix} 1.96 & -1-\tfrac{1}{2}y_2 & 0 & 0 \\ -1+\tfrac{1}{2}(y_3-y_1) & 1.96 & -1-\tfrac{1}{2}(y_3-y_1) & 0 \\ 0 & -1+\tfrac{1}{2}(y_4-y_2) & 1.96 & -1-\tfrac{1}{2}(y_4-y_2) \\ 0 & 0 & -0.6534-\tfrac{1}{2}y_3 & 1.96 \end{bmatrix}$$

To guess the initial values, we use linear interpolation, h=(ln2-0)/5≈0.14; where y_0=0, y_5=0.7. So, we get

$$\mathbf{Y}^{(0)}=\begin{bmatrix} y_1^{(0)} \\ y_2^{(0)} \\ y_3^{(0)} \\ y_4^{(0)} \end{bmatrix}=\begin{bmatrix} 0.14 \\ 0.28 \\ 0.42 \\ 0.56 \end{bmatrix}, \mathbf{J}\left(\mathbf{Y}^{(0)}\right)=\begin{bmatrix} 1.96 & -1-\tfrac{1}{2}0.28 & 0 & 0 \\ -1+\tfrac{1}{2}(0.42-0.14) & 1.96 & -1-\tfrac{1}{2}(0.42-0.14) & 0 \\ 0 & -1+\tfrac{1}{2}(0.56-0.28) & 1.96 & -1-\tfrac{1}{2}(0.56-0.28) \\ 0 & 0 & -0.6534-\tfrac{1}{2}0.42 & 1.96 \end{bmatrix}$$

$$\rightarrow \mathbf{J}\left(\mathbf{Y}^{(0)}\right)=\begin{bmatrix} 1.96 & -1.14 & 0 & 0 \\ -0.86 & 1.96 & -1.14 & 0 \\ 0 & -0.86 & 1.96 & -1.14 \\ 0 & 0 & -0.8634 & 1.96 \end{bmatrix}, \quad -\mathbf{G}\left(\mathbf{Y}^{(0)}\right)=-\begin{bmatrix} 2(0.14)-0.28-\tfrac{1}{4}0.28^2-0.2^2 0.14+0.0073 \\ -0.14+2\cdot 0.28-0.42-\tfrac{1}{4}(0.42-0.14)^2-0.2^2 0.28+0.0135 \\ -0.28+2\cdot 0.42-0.56-\tfrac{1}{4}(0.56-0.28)^2-0.2^2 0.42+0.0188 \\ -0.42+2\cdot 0.56-0.6931-\tfrac{1}{4}(0.6931-0.42)^2-0.2^2 0.56+0.0235 \end{bmatrix}=-\begin{bmatrix} -0.0179 \\ -0.0173 \\ -0.0176 \\ -0.0106 \end{bmatrix}$$

$$\begin{bmatrix} 1.96 & -1.14 & 0 & 0 \\ -0.86 & 1.96 & -1.14 & 0 \\ 0 & -0.86 & 1.96 & -1.14 \\ 0 & 0 & -0.8634 & 1.96 \end{bmatrix}\begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ h_3^{(0)} \\ h_4^{(0)} \end{bmatrix}=-\begin{bmatrix} -0.0179 \\ -0.0173 \\ -0.0176 \\ -0.0106 \end{bmatrix} \rightarrow \text{Thomas algorithm} \rightarrow \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ h_3^{(0)} \\ h_4^{(0)} \end{bmatrix}=\begin{bmatrix} 0.0414 \\ 0.0556 \\ 0.0491 \\ 0.0270 \end{bmatrix}.$$

$$\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \\ y_4^{(1)} \end{bmatrix}=\begin{bmatrix} y_1^{(0)} \\ y_2^{(0)} \\ y_3^{(0)} \\ y_4^{(0)} \end{bmatrix}+\begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ h_3^{(0)} \\ h_4^{(0)} \end{bmatrix}=\begin{bmatrix} 0.14 \\ 0.28 \\ 0.42 \\ 0.56 \end{bmatrix}+\begin{bmatrix} 0.0414 \\ 0.0556 \\ 0.0491 \\ 0.0270 \end{bmatrix}=\begin{bmatrix} 0.1814 \\ 0.3356 \\ 0.4691 \\ 0.587 \end{bmatrix}.$$

$$\mathbf{J}(\mathbf{Y}^{(k)})\mathbf{H}^{(k)}= -\mathbf{G}(\mathbf{Y}^{(k)}).$$

Ordinary differential equations (ODEs)

Finite difference method for nonlinear second-order boundary value problem

$$\mathbf{Y}^{(1)}=\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \\ y_4^{(1)} \end{bmatrix}=\begin{bmatrix} 0.1814 \\ 0.3356 \\ 0.4691 \\ 0.587 \end{bmatrix}, \mathbf{J}\left(\mathbf{Y}^{(1)}\right)=\begin{bmatrix} 1.96 & -1-\frac{1}{2}0.3356 & 0 & 0 \\ -1+\frac{1}{2}(0.4691-0.1814) & 1.96 & -1-\frac{1}{2}(0.4691-0.1814) & 0 \\ 0 & -1+\frac{1}{2}(0.587-0.3356) & 1.96 & -1-\frac{1}{2}(0.587-0.3356) \\ 0 & 0 & -0.6534-\frac{1}{2}0.4691 & 1.96 \end{bmatrix}$$

$$\to \mathbf{J}\left(\mathbf{Y}^{(1)}\right)=\begin{bmatrix} 1.96 & -1.1678 & 0 & 0 \\ -0.8562 & 1.96 & -1.1439 & 0 \\ 0 & -0.8743 & 1.96 & -1.1257 \\ 0 & 0 & -0.8880 & 1.96 \end{bmatrix}, \quad -\mathbf{G}\left(\mathbf{Y}^{(1)}\right)=-\begin{bmatrix} -0.0009 \\ 0.00004 \\ -0.00016 \\ -0.0007 \end{bmatrix}$$

$$\begin{bmatrix} 1.96 & -1.1678 & 0 & 0 \\ -0.8562 & 1.96 & -1.1439 & 0 \\ 0 & -0.8743 & 1.96 & -1.1257 \\ 0 & 0 & -0.8880 & 1.96 \end{bmatrix}\begin{bmatrix} h_1^{(1)} \\ h_2^{(1)} \\ h_3^{(1)} \\ h_4^{(1)} \end{bmatrix}=-\begin{bmatrix} -0.0009 \\ 0.00004 \\ -0.00016 \\ -0.0007 \end{bmatrix} \to \text{Thomas algorithm} \to \begin{bmatrix} h_1^{(1)} \\ h_2^{(1)} \\ h_3^{(1)} \\ h_4^{(1)} \end{bmatrix}=\begin{bmatrix} 0.0011 \\ 0.0010 \\ 0.0010 \\ 0.0008 \end{bmatrix}.$$

$$\begin{bmatrix} y_1^{(2)} \\ y_2^{(2)} \\ y_3^{(2)} \\ y_4^{(2)} \end{bmatrix}=\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \\ y_4^{(1)} \end{bmatrix}+\begin{bmatrix} h_1^{(1)} \\ h_2^{(1)} \\ h_3^{(1)} \\ h_4^{(1)} \end{bmatrix}=\begin{bmatrix} 0.1814 \\ 0.3356 \\ 0.4691 \\ 0.587 \end{bmatrix}+\begin{bmatrix} 0.0011 \\ 0.0010 \\ 0.0010 \\ 0.0008 \end{bmatrix}=\begin{bmatrix} 0.1825 \\ 0.3366 \\ 0.4701 \\ 0.5878 \end{bmatrix}.$$

Stopping criterion: *maximum-magnitude* norm of increment solution vector < ε=0.02. $\left\|\mathbf{Y}^{(2)}-\mathbf{Y}^{(1)}\right\|_\infty=\left\|\mathbf{H}^{(1)}\right\|_\infty=0.0011<\varepsilon$.

The final solution is

$$\begin{bmatrix} y_1^{(2)} \\ y_2^{(2)} \\ y_3^{(2)} \\ y_4^{(2)} \end{bmatrix}=\begin{bmatrix} 0.1825 \\ 0.3366 \\ 0.4701 \\ 0.5878 \end{bmatrix}. \quad \textit{exact solution}: \begin{bmatrix} \ln 1.2 \\ \ln 1.4 \\ \ln 1.6 \\ \ln 1.8 \end{bmatrix}=\begin{bmatrix} 0.1823 \\ 0.3365 \\ 0.4700 \\ 0.5878 \end{bmatrix}.$$

Note: If the problem is simplified by only finding 2 points (y_1 and y_2), Then Thomas algorithm is not required since the matrix is 2×2. Use the below simple formula.

$$\mathbf{J}^{-1}=\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1}=\frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}. \to \quad \mathbf{H}=\mathbf{J}^{-1}(-\mathbf{G}).$$

Ordinary differential equations (ODEs)

Finite difference & Simpson method for fundamental solution – Dirac Delta function

$$\frac{d^2}{dx^2}G(x)=\delta(x) \quad \Longrightarrow \quad \frac{d}{dx}G(x)=H(x)+C$$

$$\frac{d}{dx}H(x)=\delta(x)$$

$$\delta(x)=\begin{cases}0, & x\neq 0\\ \infty, & x=0\end{cases}$$

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)dx=f(a),$$

$$H(x-a)=\begin{cases}0, & x<a\\ 1, & x\geq a\end{cases}$$

$$\int_0^x \delta(s-a)ds=H(x-a)$$

$$\to \delta(x-a)=\frac{d}{dx}H(x-a)$$

where $H(x)$ is Heaviside function, for convenience, we can set constant such as

$$G(x)=xH(x)-\tfrac{1}{2}x=\tfrac{1}{2}|x|$$

Let $\frac{d^2}{dx^2}u(x)=\sin(x)$

$$\int_\Omega G(x-y)u''(x)dx=G(x-y)u'(x)\Big|_{x=a}^{b}-\int_\Omega G'(x-y)u'(x)dx$$

$$\int_\Omega G(x-y)u''(x)dx=G(x-y)u'(x)\Big|_a^b-G'(x-y)u(x)\Big|_a^b+\int_\Omega G''(x-y)u(x)dx$$

Let the boundary→0 (subjects to conditions)

$$\int_\Omega \tfrac{1}{2}|x-y|\sin(x)dx=0-0+\int_\Omega \delta(x-y)u(x)dx=u(y)$$

Newton forward interpolation:

$$f(x)=f_0+\frac{(x-x_0)}{h}\Delta f_0+\frac{1}{2!}(x-x_0)(x-x_0-h)\frac{\Delta^2 f_0}{h^2}$$
$$+\frac{1}{3!}(x-x_0)(x-x_0-h)(x-x_0-2h)\frac{\Delta^3 f_0}{h^3}+O(h^4)$$

$$f_0^{(3)}=\frac{\Delta^3 f_0}{h^3}+O(h),\ f_0^{(2)}=\frac{\Delta^2 f_0}{h^2}-hf_0^{(3)}+O(h^2)$$

$$f_0^{(1)}=\frac{\Delta f_0}{h}-\frac{1}{2!}hf_0^{(2)}-\frac{1}{3!}h^2 f_0^{(3)}-O(h^3)$$

Let $rh=x-x_0$, we get

$$f(x)=f_0+r\Delta f_0+\frac{r(r-1)}{2!}\Delta^2 f_0+\frac{r(r-1)(r-2)}{3!}\Delta^3 f_0+O(h^4)$$

$$\Delta^0 f_i=f_i,\quad \Delta^k f_i=\Delta^{k-1}f_{i+1}-\Delta^{k-1}f_i$$

$$\Delta f_0=f_1-f_0,\ \Delta^2 f_0=f_2-2f_1+f_0$$

$$\Delta^3 f_0=f_3-3f_2+3f_1-f_0$$

Taylor series

$$f(x)=f_0+(x-x_0)f_0^{(1)}+\frac{1}{2!}(x-x_0)^2 f_0^{(2)}+\frac{1}{3!}(x-x_0)^3 f_0^{(3)}+O\left((x-x_0)^4\right)$$

Ordinary differential equations (ODEs)

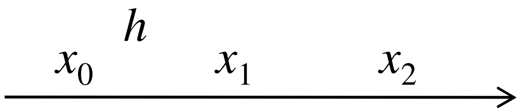
Finite difference & Simpson method for fundamental solution – Dirac Delta function

$$f(x) = f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + \frac{r(r-1)(r-2)}{3!}\Delta^3 f_0 + O(h^4)$$

Simpson method

$$\int_{x_0}^{x_2} f(x)dx = \int_{x_0}^{x_2} f_0 + r\Delta f_0 + \frac{r(r-1)}{2!}\Delta^2 f_0 + O(h^3)dx$$

$$= \frac{h}{3}[f_0 + 4f_1 + f_2] + 2hO(h^3) = \frac{h}{3}[f_0 + 4f_1 + f_2] + O(h^4)$$

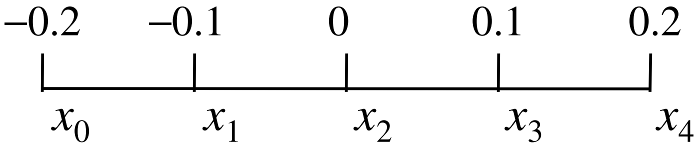

h

x_0 x_1 x_2

E.g. : **Laplace problem**:

$$\frac{d^2}{dx^2}u(x) = \delta(x-0)$$

Fundamental solution


-0.2 -0.1 0 0.1 0.2

x_0 x_1 x_2 x_3 x_4

BC: $u(x_0)=u_0=$ ½|–0.2|=0.1, $u_4=0.1$

Exact: $u(x)=$ ½|x|

$$\frac{d^2}{dx^2}u(x_i) = \delta(x_i) \rightarrow \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \delta_i$$

Let i=1, $$\frac{u_2 - 2u_1 + u_0}{h^2} = \delta_1 \rightarrow \begin{bmatrix} -\frac{2}{h^2} & \frac{1}{h^2} & 0 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = 0 - \frac{u_0}{h^2}$$

Let i=3, $$\frac{u_4 - 2u_3 + u_2}{h^2} = \delta_3 \rightarrow \begin{bmatrix} 0 & \frac{1}{h^2} & -\frac{2}{h^2} \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = 0 - \frac{u_4}{h^2}$$

$$\rightarrow \begin{bmatrix} -2/h^2 & 1/h^2 & 0 \\ 0 & 1/h^2 & -2/h^2 \\ 2/h^2 & -6/h^2 & 2/h^2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} -1/h \\ -1/h \\ 1/h \end{bmatrix}$$

⇩

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 0.0625 \\ 0.025 \\ 0.0625 \end{bmatrix}$$

$$\int_{x_1}^{x_3} \frac{d^2}{dx^2}u(x)dx = \int_{x_1}^{x_3} \delta(x-0)dx = 1,$$

$$\frac{h}{3}[u_1'' + 4u_2'' + u_3''] = 1.$$

$$\rightarrow \begin{bmatrix} \frac{2}{h^2} & \frac{-6}{h^2} & \frac{2}{h^2} \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \frac{3h - u_0 - u_4}{h^2}$$

⇨ $$\frac{u_2 - 2u_1 + u_0}{h^2} + 4\frac{u_3 - 2u_2 + u_1}{h^2} + \frac{u_4 - 2u_3 + u_2}{h^2} = \frac{3}{h}$$

If u_i'' involve ghost node, use $u_i''=\delta(x-0)$ to calculate ghost u node value.

Or (last choice) use $u_i'=\mathrm{H}(x-0)$ to calculate ghost u node value.

Partial differential equation : von Neumann Stability Analysis

- Provides a systematic method for determining stability → von Neumann Stability Analysis
- Provides insight into discretization errors

Fourier mode: $\Phi_k(x)=e^{i2\pi kx}$, $k\in Z$ (integer)

-Periodic (period=1), $\Phi_k(x)=\Phi_k(x+1)$

-Orthogonality $\int_0^1 \Phi_k(x)\Phi_{-k'}(x)dx = \delta_{kk'}$

-Eigenfunction of $\partial^m/\,\partial x^m$ $\frac{\partial^m}{\partial x^m}\Phi_k(x) = (i2\pi k)^m\,\Phi_k(x)$

Form a basis for periodic functions in $L^2([0,1])$

$$v(x) = \sum_{k=-\infty}^{\infty} V_k \Phi_k(x) = \sum_{k=-\infty}^{\infty} V_k e^{i2\pi kx}$$

Parseval's theorem

$$\|v\|_2^2 = \sum_{k=-\infty}^{\infty} |V_k|^2$$

Partial differential equation : von Neumann Stability Analysis

Fourier Analysis : wave equation

$$u(x,t)=\sum_{k=-\infty}^{\infty}U_k(t)\Phi_k(x)=\sum_{k=-\infty}^{\infty}U_k(t)e^{i2\pi kx}$$

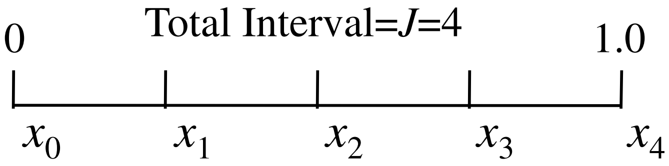
$$u_t+Wu_x=0 \;\rightarrow\; \sum_{k=-\infty}^{\infty}\left(\frac{dU_k}{dt}+i2\pi kWU_k\right)e^{i2\pi kx}=0 \;\Rightarrow\; \frac{dU_k}{dt}+i2\pi kWU_k=0$$

$$\Downarrow$$

$$u(x,0)=u^0(x)=\sum_{k=-\infty}^{\infty}U_k(0)e^{i2\pi kx}=\sum_{k=-\infty}^{\infty}U_k^0e^{i2\pi kx} \;\Rightarrow\; U_k(t)=U_k^0e^{-i2\pi kWt}$$

Fourier mode: $\Phi_k(x)=e^{i2\pi kx}$, $k\in Z$ (integer) $\rightarrow$ $\mathbf{\Phi}_k=[\Phi_k(x_0)\ \ldots\Phi_k(x_{J-1})]^T$, $k\in(-J/2+1, J/2)$

J+1 equally spaced nodes in domain, only J unique value (periodic, $x_0=x_J$). So, only J terms in Fourier series used to describe a FD FD solution on a periodic domain with J+1 points.



$\Phi_k(x_j)=e^{i2\pi kj\Delta x}=e^{ij\theta}=\Phi_{kj}$, where $\theta=2\pi k\Delta x$.

$j\in(0,\ldots, J-1=3)$

$k\in(-J/2+1, J/2)=(-1,\ldots, 2)$

$x_j=j\Delta x$, $\Delta x=1/J$

$k\in(-J/2+1, J/2)\rightarrow\theta\in(-\pi+2\pi\Delta x, \pi)$

-periodic (period= J)

-Orthogonality

$$\frac{1}{J}\mathbf{\Phi}_\theta^T\mathbf{\Phi}_{-\theta'}=\frac{1}{J}\sum_{j=0}^{J-1}e^{i2\pi kj\Delta x}e^{-i2\pi k'j\Delta x}=\delta_{kk'}$$

$$=\frac{1}{J}\sum_{j=0}^{J-1}e^{ij\theta}e^{-ij\theta'}=\begin{cases}1 & ,\theta=\theta'\\ 0 & ,\theta\neq\theta'\end{cases}$$

Partial differential equation : von Neumann Stability Analysis

Fourier Analysis : wave equation

Finite difference:

$\Delta_h\,[f](x)=f(x+h)-f(x)$,

$\nabla_h\,[f](x)=f(x)-f(x-h)$,

$\delta_h\,[f](x)=f(x+\tfrac{1}{2}h)-f(x-\tfrac{1}{2}h)$.

$$f''(x)\approx\frac{\delta_h^2[f](x)}{h^2}=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

$$f''(x)\approx\frac{\Delta_h^2[f](x)}{h^2}=\frac{f(x+2h)-2f(x+h)+f(x)}{h^2}$$

$\Phi_k(x_j)=e^{i2\pi kj\Delta x}=e^{ij\theta}=\Phi_{kj}=\Phi_{\theta j}$, where $\theta=2\pi k\Delta x$.

$e^{ij\theta}=\cos(j\theta)+i\sin(j\theta)$

Eigenfunctions of difference operators:

$$\delta_{2\Delta x}\Phi_{\theta j}=\Phi_{\theta(j+1)}-\Phi_{\theta(j-1)}=$$
$$=[\cos\theta(j+1)+i\sin\theta(j+1)]-[\cos\theta(j-1)+i\sin\theta(j-1)]$$
$$=[\cos\theta(j+1)-\cos\theta(j-1)]+i[\sin\theta(j+1)-\sin\theta(j-1)]$$
$$=-2\sin((2\theta j)/2)\sin((2\theta)/2)+i\,2\cos((2\theta j)/2)\sin((2\theta)/2)$$
$$=2i\sin\theta\,[\cos\theta j+i\sin\theta j]\,]=2i\sin\theta\,\Phi_{\theta j}$$

$$\delta^2_{\Delta x}\Phi_{\theta j}=\exp(i\theta(j+1))-2\exp(i\theta j)+\exp(i\theta(j-1))$$
$$=[\exp(i\theta)-2+\exp(-i\theta)]\exp(i\theta j)$$
$$=[2\cos(\theta)-2]\,\Phi_{\theta j}=-4\sin^2(\theta/2)\,\Phi_{\theta j}.$$

$$\Delta^-_{\Delta x}\Phi_{\theta j}=\exp(i\theta j)-\exp(i\theta(j-1))$$
$$=[1-\exp(-i\theta)]\,\Phi_{\theta j}.$$

Trigo formulae

$\sin(a\pm b)=\sin(a)\cos(b)\pm\cos(a)\sin(b)$

$\cos(a\pm b)=\cos(a)\cos(b)-+\sin(a)\sin(b)$

$\sin(a)-\sin(b)=2\cos((a+b)/2)\sin((a-b)/2)$

$\cos(a)-\cos(b)=-2\sin((a+b)/2)\sin((a-b)/2)$

For simplicity, sometime is written as:

$$\delta_{2x}\Phi_{\theta j}=\Phi_{\theta(j+1)}-\Phi_{\theta(j-1)}=2i\sin\theta\,\Phi_{\theta j}$$
$$\delta^2_x\Phi_{\theta j}=\Phi_{\theta(j+1)}-2\Phi_{\theta(j)}+\Phi_{\theta(j-1)}=$$
$$=-4\sin^2(\theta/2)\,\Phi_{\theta j}.$$
$$\Delta^-_x\Phi_{\theta j}=\Phi_{\theta j}-\Phi_{\theta(j-1)}=[1-\exp(-i\theta)]\,\Phi_{\theta j}.$$

Fourier Analysis

$\delta_{2x}\,\Phi_{\theta j} = \Phi_{\theta\,(j+1)} - \Phi_{\theta\,(j-1)} = 2\mathrm{i}\,\sin\theta\,\Phi_{\theta j}$
$\delta^2_{x}\,\Phi_{\theta j} = \Phi_{\theta\,(j+1)} - 2\Phi_{\theta\,(j)} + \Phi_{\theta\,(j-1)} =$
$= -4\sin^2(\theta/2)\,\Phi_{\theta j}.$
$\Delta^-_x\Phi_{\theta j} = \Phi_{\theta j} - \Phi_{\theta\,(j-1)} = [1-\exp(-\mathrm{i}\theta)]\,\Phi_{\theta j}.$

First order upwind scheme

$$u_j^n = \sum_\theta U_\theta^n \Phi_{\theta j} = \sum_\theta U_\theta^n e^{ij\theta}$$

$u_t + Wu_x = 0 \rightarrow \Delta_t\, u_j^n/\Delta t + W\Delta^-_x u_j^n/\Delta x = 0 \rightarrow u_j^{n+1} - u_j^n + C(u_j^n - u_{j-1}^n) = 0,\ \forall j$ where $C = W\,\Delta t/\Delta x$.

$$\sum_\theta \left(U_\theta^{n+1} - U_\theta^n + C\left(1-e^{-i\theta}\right)U_\theta^n\right)e^{ij\theta} = 0,\ \forall j \quad\Longrightarrow\quad U_\theta^{n+1} = \left(\left(1-C\right)+Ce^{-i\theta}\right)U_\theta^n = \underbrace{g\left(C,\theta\right)}_{\text{Amplification factor}}U_\theta^n$$

This scheme is stable if $|U_\theta^{n+1}| \le |U_\theta^n|,\ \forall\theta$ which implies $|g(C,\theta)| \le 1,\ \forall\theta$

Stable if
$|g(C,\theta)| \le 1 \rightarrow 0 \le C = W\Delta t/\Delta x \le 1$

$|g(C,\theta)|^2 = |(1-C)+Ce^{-i\theta}|^2 = (1-C+C\cos\theta)^2 + C^2\sin^2(\theta)$
$= (1-2C\sin^2(\theta/2))^2 + 4C^2\sin^2(\theta/2)\cos^2(\theta/2)$
$= 1-4C(1-C)\sin^2(\theta/2).$ $1-4C(1-C)\sin^2(\theta/2) \le 1 \rightarrow C(1-C) \ge 0 \rightarrow 0 \le C \le 1$ (since $\sin^2 \ge 0$)

FTCS scheme (Forward-Time Central-Space)

$u_t + Wu_x = 0 \rightarrow \Delta_t\, u_j^n/\Delta t + W\,\delta_{2x}\, u_j^n/2\Delta x = 0 \rightarrow u_j^{n+1} - u_j^n + C/2(u_{j+1}^n - u_{j-1}^n) = 0,\ \forall j$ where $C = W\,\Delta t/\Delta x$.

$$\sum_\theta \left(U_\theta^{n+1} - U_\theta^n + iC\sin(\theta)U_\theta^n\right)e^{ij\theta} = 0,\ \forall j \quad\Longrightarrow\quad U_\theta^{n+1} = \left(1-iC\sin(\theta)\right)U_\theta^n = \underbrace{g\left(C,\theta\right)}_{\text{Amplification factor}}U_\theta^n$$

$|g(C,\theta)|^2 = |1-\mathrm{i}C\sin\theta|^2 = 1+C^2\sin^2(\theta) \ge 1,$ for $C \neq 0$.

$\Longrightarrow$ This scheme is unconditionally unstable → Not convergent

Partial differential equations (PDEs)

Introduction – Finite Difference Method

The general second-order PDE is given

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu=G\,,\ or\quad Au_{xx}+Bu_{xy}+Cu_{yy}+Du_x+Eu_y+Fu=G$$

where u, A, B, C, D, E, F and G are functions of x and y.

The PDE is called $\begin{Bmatrix} elliptic \\ parabolic \\ hyperbolic \end{Bmatrix}$ $if\ \left(B^2-4AC\right)\begin{cases} <0 \\ =0 \\ >0 \end{cases}$

e.g.

1. Laplace equation: $u(x,y)$ $\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$ A=C=1, B=0 → B^2-4AC=0-4(1)(1)=-4<0 →elliptic equation
2. Heat equation: $u(x,t)$ $\frac{\partial^2 u}{\partial x^2}-\frac{1}{c^2}\frac{\partial u}{\partial t}=0$ A=1, B=C=0 → B^2-4AC=0 →parabolic equation
3. Wave equation: $u(x,t)$ $\frac{\partial^2 u}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2}=0$ A=1, B=0, C=-1/c^2 → B^2-4AC=0-4(1)(-1/c^2)=4/c^2>0 →hyperbolic equation

Let u_{ij} is the approximation for $u(x_i,y_j)$, then we get

$$\left(\frac{\partial u}{\partial x}\right)_{i,j}=\frac{u_{i+1,j}-u_{i,j}}{h}+O(h)\quad [forward\ difference],\quad \left(\frac{\partial u}{\partial x}\right)_{i,j}=\frac{u_{i,j}-u_{i-1,j}}{h}+O(h)\quad [backward\ difference]$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j}=\frac{u_{i+1,j}-u_{i-1,j}}{2h}+O(h^2)\quad [central\ difference],\quad \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}+O(h^2)\quad [central\ difference]$$

$$same\ approach\ for:\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j}=\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2}+O(k^2)\,,\cdots\quad where\ h=\Delta x,k=\Delta y=\Delta t.$$

Partial differential equations (PDEs)

Hyperbolic equation : Wave equation

The general wave equation is given

$$u_{tt}=c^2u_{xx}, \qquad 0<x<a,\ \ 0<t<T,$$

where c is constant, with boundary condition

$$u(0,t)=\mathrm{u}(a,t)=0, \qquad 0<t<T,$$

and initial value condition

$$u(x,0)=f(x), \qquad 0\le x\le l, \qquad \text{(initial displacement)}$$

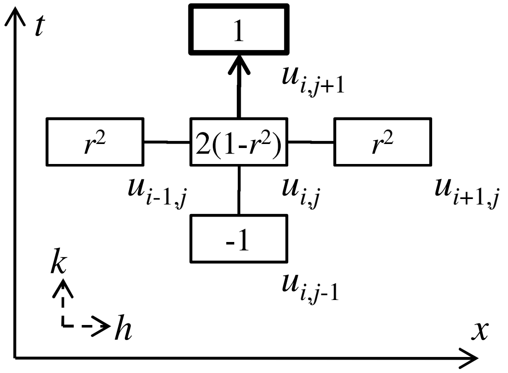
$$u_t(x,0)=g(x), \qquad 0\le x\le l. \qquad \text{(initial velocity)}$$

At point (x_i,t_j) with $h=\Delta x$, $k=\Delta t$, we get $\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j}=c^2\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \rightarrow \frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2}=c^2\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}$

Now, let $r=ck/h$, we get $u_{i,j+1}-2u_{i,j}+u_{i,j-1}=r^2\left(u_{i+1,j}-2u_{i,j}+u_{i-1,j}\right) \rightarrow u_{i,j+1}=2\left(1-r^2\right)u_{i,j}-u_{i,j-1}+r^2u_{i+1,j}+r^2u_{i-1,j}$

Finally, we get $\boxed{u_{i,j+1}=r^2u_{i-1,j}+2\left(1-r^2\right)u_{i,j}+r^2u_{i+1,j}-u_{i,j-1}}$

The **computational grid** (explicit) is given:



Partial differential equations (PDEs)

Hyperbolic equation : Wave equation

e.g. A wave equation is given

$u_{tt}=u_{xx}$, $0<x<1$, $0<t<0.2$,

with boundary condition

$u(0,t)=\mathrm{u}(1,t)=0$, $0<t<0.2$,

and initial value condition

$u(x,0)= \frac{1}{8}\sin(\pi x)$, $0\le x\le 1$, (initial displacement)

$u_t(x,0)=0$, $0\le x\le 1$. (initial velocity)

Solve the above use finite difference method for x=0(0.2)1 and t=0(0.1)0.2. All the calculation use 4 decimal point(4DP). Exact solution is: $u(x,t)={}^1/_8\sin(\pi x)\cos(\pi t)$.

Solution:

With $h=\Delta x=0.2$, $k=\Delta t=0.1$, x-axis : $x_0=0$, $x_1=0.2$, $x_2=0.4$, $x_3=0.6$, $x_4=0.8$, $x_5=1$.

t-axis : $t_0=0$, $t_1=0.1$, $t_2=0.2$.

Given $u(0,t)=0$ and $u(1,t)=0$ for $0\le t \le 0.2$, so we get

$u_{0,0}=u(0,0)=0$, $u_{0,1}=u(0,0.1)=0$, $u_{0,2}=u(0,0.2)=0$. And,

$u_{5,0}=u(1,0)=0$, $u_{5,1}=u(1,0.1)=0$, $u_{5,2}=u(1,0.2)=0$.

Given $u(x,0)= \frac{1}{8}\sin(\pi x)$, $0\le x\le 1$, so we get

$u_{0,0}=u(x_0,t_0)=u(0,0)= \frac{1}{8}\sin(\pi\times 0)=0$,

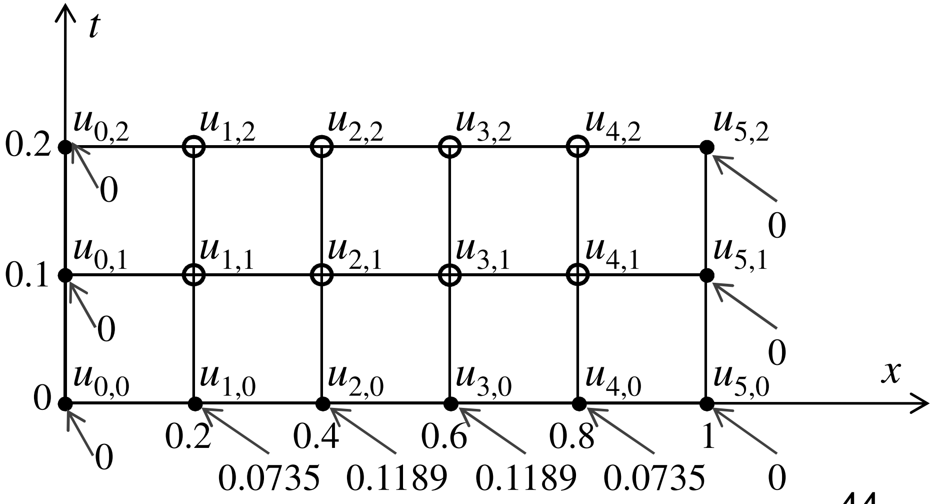
$u_{1,0}=u(x_1,t_0)=u(0.2,0)= \frac{1}{8}\sin(\pi\times 0.2)=0.0735$,

$u_{2,0}=u(x_2,t_0)=u(0.4,0)= \frac{1}{8}\sin(\pi\times 0.4)=0.1189$,

$u_{3,0}=u(x_3,t_0)=u(0.6,0)= \frac{1}{8}\sin(\pi\times 0.6)=0.1189$,

$u_{4,0}=u(x_4,t_0)=u(0.8,0)= \frac{1}{8}\sin(\pi\times 0.8)=0.0735$,

$u_{5,0}=u(x_5,t_0)=u(1,0)= \frac{1}{8}\sin(\pi\times 1)=0$.



Partial differential equations (PDEs)

Hyperbolic equation : Wave equation

Given $u_t(x,0)=0$ for $0 \le x \le 1$. So we get $\frac{\partial u}{\partial t}(x_i,0)=0, \quad \frac{\partial u}{\partial t}(x_i,t_0)=0, \quad \rightarrow \frac{\partial u_{i,0}}{\partial t}=0 \quad \rightarrow \frac{u_{i,1}-u_{i,-1}}{2k}=0.$
or $u_{i,-1}=u_{i,1}$

So, we get $u_{0,-1}=u_{0,1}$; $u_{1,-1}=u_{1,1}$; $u_{2,-1}=u_{2,1}$; $u_{3,-1}=u_{3,1}$; $u_{4,-1}=u_{4,1}$; $u_{5,-1}=u_{5,1}$.

By observing the above values, the problem is symmetry on $x=½$.

So, we only need to calculate for $u_{1,1}$, $u_{2,1}$, $u_{3,1}$, $u_{4,1}$, $u_{1,2}$, $u_{2,2}$, $u_{3,2}$, and $u_{4,2}$.

At point (x_i,t_j) we get

$$\left(\frac{\partial^2 u_{i,j}}{\partial t^2}\right)=\left(\frac{\partial^2 u_{i,j}}{\partial x^2}\right)\rightarrow \quad \frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2}-\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}=0, \quad let\ r=k/h=0.1/0.2=½,$$

$$u_{i,j+1}-2u_{i,j}+u_{i,j-1}=r^2\left(u_{i+1,j}-2u_{i,j}+u_{i-1,j}\right)\rightarrow \quad u_{i,j+1}=r^2u_{i-1,j}+2\left(1-r^2\right)u_{i,j}+r^2u_{i+1,j}-u_{i,j-1}$$

Finally, we get $$\boxed{u_{i,j+1}=\tfrac{1}{4}\left(u_{i-1,j}+6u_{i,j}+u_{i+1,j}\right)-u_{i,j-1} \quad (\text{explicit method})}$$

For i=1, j=0;

$u_{1,1}$=¼($u_{0,0}$+6$u_{1,0}$ +$u_{2,0}$)- $u_{1,-1}$ =¼($u_{0,0}$+6$u_{1,0}$+$u_{2,0}$)- $u_{1,1}$,

2$u_{1,1}$=¼($u_{0,0}$+6$u_{1,0}$+$u_{2,0}$)=¼(0+6[0.0735]+0.1189)=0.1400

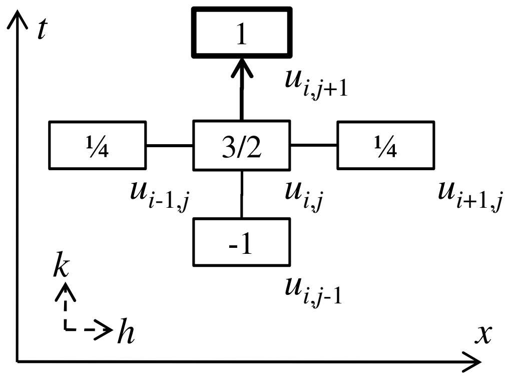
$u_{1,1}$=0.0700

For i=2, j=0;

$u_{2,1}$=¼($u_{1,0}$+6$u_{2,0}$ +$u_{3,0}$)- $u_{2,-1}$ =¼($u_{1,0}$+6$u_{2,0}$+$u_{3,0}$)- $u_{2,1}$,

2$u_{2,1}$=¼($u_{1,0}$+6$u_{2,0}$+$u_{3,0}$)=¼(0.0735+6[0.1189]+0.1189)=0.2265

$u_{2,1}$=0.1132



Computational grid - explicit

Partial differential equations (PDEs)

Hyperbolic equation : Wave equation

For i=3, j=0;

$u_{3,1}$=¼($u_{2,0}$+6$u_{3,0}$ +$u_{4,0}$)- $u_{3,-1}$ =¼($u_{2,0}$+6$u_{3,0}$+$u_{4,0}$)- $u_{3,1}$,

2$u_{3,1}$=¼($u_{2,0}$+6$u_{3,0}$+$u_{4,0}$)=¼(0.1189+6[0.1189]+0.0735)=0.2265 → $u_{3,1}$=0.1132

For i=4, j=0;

$u_{4,1}$=¼($u_{3,0}$+6$u_{4,0}$ +$u_{5,0}$)- $u_{4,-1}$ =¼($u_{3,0}$+6$u_{4,0}$+$u_{5,0}$)- $u_{4,1}$,

2$u_{4,1}$=¼($u_{3,0}$+6$u_{4,0}$+$u_{5,0}$)=¼(0.1189+6[0.0735]+0)=0.1400 → $u_{4,1}$=0.0700

For i=1, j=1;

$u_{1,2}$=¼($u_{0,1}$+6$u_{1,1}$ +$u_{2,1}$)- $u_{1,0}$=¼(0+6[0.0700]+0.1132)- 0.0735=0.0598

For i=2, j=1;

$u_{2,2}$=¼($u_{1,1}$+6$u_{2,1}$ +$u_{3,1}$)- $u_{2,0}$=¼(0.0700+6[0.1132]+0.1132)- 0.1189=0.0967

For i=3, j=1;

$u_{3,2}$=¼($u_{2,1}$+6$u_{3,1}$ +$u_{4,1}$)- $u_{3,0}$=¼(0.1132+6[0.1132]+0.0700)- 0.1189=0.0967

For i=4, j=1;

$u_{4,2}$=¼($u_{3,1}$+6$u_{4,1}$ +$u_{5,1}$)- $u_{4,0}$=¼(0.1132+6[0.0700]+0)- 0.0735=0.0598

The solutions are: (symmetry on x= ½)

u(0.2,0.1)≈$u_{1,1}$=0.0700; u(0.4,0.1)≈$u_{2,1}$=0.1132; u(0.6,0.1)≈$u_{3,1}$=0.1132; u(0.8,0.1)≈$u_{4,1}$=0.0700;

u(0.2,0.2)≈$u_{1,2}$=0.0598; u(0.4,0.2)≈$u_{2,2}$=0.0967; u(0.6,0.2)≈$u_{3,2}$=0.0967; u(0.8,0.2)≈$u_{4,2}$=0.0598;

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

The Laplace equation is given

$$u_{xx}+u_{yy}=0 \text{ , or } \nabla^2 u=0, \qquad 0<x<a,\ 0<y<b,$$

with boundary conditions

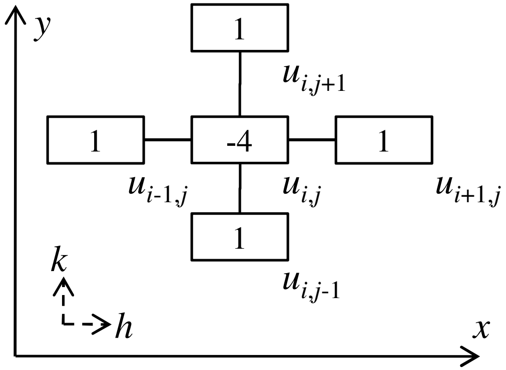
$$u(x,0)=f_1(x) \text{ and } u(x,b)=f_2(x), \qquad 0\le x\le a,$$
$$u(0,y)=g_1(y) \text{ and } u(a,y)=g_2(y), \qquad 0\le y\le b.$$

The above boundary conditions is called Dirichlet problem.

At point (x_i,y_j) with $h=\Delta x$, $k=\Delta y$, we get $\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}+\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j}=0 \rightarrow \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}+\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2}=0$

Now, let $h=k$, we get $\boxed{u_{i,j-1}+u_{i-1,j}-4u_{i,j}+u_{i+1,j}+u_{i,j+1}=0}$

We will get the final form of linear system, **Au=b** with **A** is strictly diagonally dominant matrix. $|a_{ii}|> \sum_{j=1}^{n} |a_{ij}|$, $j\neq i$. (row summation).
The linear system with strictly diagonally matrix can be solved using Gauss-Seidel iteration or
SOR (successive over-relaxation) method.



Computational grid - implicit

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Gauss-Seidel iteration and Successive over-relaxation (SOR)

For general matrix $\mathbf{A}_{n\times n}$, we get

$$\mathbf{Ax=b}$$

Using the splitting matrix, **Q**, we get

$$\mathbf{Qx=(Q\text{-}A)x+b}$$

or can be written iterative process as

$$\mathbf{Qx}^{(k)}= (\mathbf{Q}\text{-}\mathbf{A})\mathbf{x}^{(k\text{-}1)}+\mathbf{b},\ \ (k\geq 1) \qquad (a)$$

The initial vector $\mathbf{x}^{(0)}$ can be arbitrary. An iterative method in equation (*a*) converges if it converges for Any initial vector $\mathbf{x}^{(0)}$.

Let $\mathbf{A=D+L}_s\mathbf{+U}_s$, where $\mathbf{D}$=diag($\mathbf{A}$), $\mathbf{L}_s(\mathbf{U}_s)$ is strictly lower(upper) triangular part of **Q**.

Iteration process in (a) is called:

- Richardson method: if $\mathbf{Q=I}_{n\times n}$,
- Jacobi method: if $\mathbf{Q=D}$,
- **Gauss-Seidel method**: if $\mathbf{Q=D+L}_s$,

  $(a)\rightarrow (\mathbf{D+L}_s)\mathbf{x}^{(k)}= (\mathbf{D+L}_s\text{-}(\mathbf{D+L}_s\mathbf{+U}_s))\mathbf{x}^{(k\text{-}1)}\mathbf{+b} \rightarrow \boxed{(\mathbf{D+L}_s)\mathbf{x}^{(k)}= \text{-}\mathbf{U}_s\mathbf{x}^{(k\text{-}1)}\mathbf{+b}}$
- **SOR method**: if $\mathbf{Q}=\omega^{-1}(\mathbf{D}+\omega\mathbf{L}_s)$,

  $(a)\rightarrow (\omega^{-1}(\mathbf{D}+\omega\mathbf{L}_s))\mathbf{x}^{(k)}= (\omega^{-1}(\mathbf{D}+\omega\mathbf{L}_s)\text{-}(\mathbf{D+L}_s\mathbf{+U}_s))\mathbf{x}^{(k\text{-}1)}\mathbf{+b} \rightarrow \boxed{(\mathbf{D}+\omega\mathbf{L}_s)\mathbf{x}^{(k)}= -\ \omega\mathbf{U}_s\mathbf{x}^{(k\text{-}1)}+\omega\mathbf{b}+(1\text{-}\omega)\mathbf{Dx}^{(k\text{-}1)}}$

  (note: if ω=1, then SOR is identical to G-S method.

  the parameter in the range $0<\omega<1$ if the system is not convergent by Gauss-Siedel method. The parameter in the range $1<\omega<2$ will accelerate the convergence of Gauss-Seidel method.

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Gauss-Seidel iteration and Successive over-relaxation (SOR)

Gauss-Seidel method: $\boxed{(\mathbf{D}+\mathbf{L}_s)\mathbf{x}^{(k)}= -\mathbf{U}_s\mathbf{x}^{(k-1)}+\mathbf{b}}$ **SOR method**: $\boxed{(\mathbf{D}+\omega\mathbf{L}_s)\mathbf{x}^{(k)}= -\ \omega\mathbf{U}_s\mathbf{x}^{(k-1)}+\omega\mathbf{b}+(1-\omega)\mathbf{D}\mathbf{x}^{(k-1)}}$

E.g. solve the below system with initial value $\mathbf{x}^{(0)}=(0,0,0)^T$ using Gauss-Seidel method and SOR (ω=0.85).

$$\mathbf{Ax}=\mathbf{b} \quad \rightarrow \quad \begin{bmatrix} 2 & -1 & 0 \\ 1 & 6 & -2 \\ 4 & -3 & 8 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}=\begin{bmatrix} 2 \\ -4 \\ 5 \end{bmatrix}$$

So, we get

$$\mathbf{D}=\begin{bmatrix} 2 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 8 \end{bmatrix}, \quad \mathbf{L}_s=\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 4 & -3 & 0 \end{bmatrix}, \quad \mathbf{U}_s=\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -2 \\ 0 & 0 & 0 \end{bmatrix} \rightarrow \mathbf{A}=\mathbf{D}+\mathbf{L}_s+\mathbf{U}_s$$

G-S:

$$\begin{bmatrix} 2 & 0 & 0 \\ 1 & 6 & 0 \\ 4 & -3 & 8 \end{bmatrix}\mathbf{x}^{(k)}=-\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -2 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{x}^{(k-1)}+\begin{bmatrix} 2 \\ -4 \\ 5 \end{bmatrix} \quad \rightarrow$$

$$\begin{aligned} x_1^{(k)} &= \tfrac{1}{2}x_2^{(k-1)}+\tfrac{2}{2}, \\ x_2^{(k)} &= \tfrac{1}{6}\left(-x_1^{(k)}+2x_3^{(k-1)}-4\right)=-\tfrac{1}{6}x_1^{(k)}+\tfrac{1}{3}x_3^{(k-1)}-\tfrac{2}{3}, \\ x_3^{(k)} &= \tfrac{1}{8}\left(-4x_1^{(k)}+3x_2^{(k)}+5\right)=-\tfrac{1}{2}x_1^{(k)}+\tfrac{3}{8}x_2^{(k)}+\tfrac{5}{8}, \end{aligned}$$

SOR:

$$\begin{bmatrix} 2 & 0 & 0 \\ 0.85(1) & 6 & 0 \\ 0.85(4) & 0.85(-3) & 8 \end{bmatrix}\mathbf{x}^{(k)}=-\begin{bmatrix} 0 & 0.85(-1) & 0 \\ 0 & 0 & 0.85(-2) \\ 0 & 0 & 0 \end{bmatrix}\mathbf{x}^{(k-1)}+\begin{bmatrix} 0.85(2) \\ 0.85(-4) \\ 0.85(5) \end{bmatrix}+(0.15)\begin{bmatrix} 2 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 8 \end{bmatrix}\mathbf{x}^{(k-1)}$$

$$\rightarrow \quad \begin{aligned} x_1^{(k)} &= \tfrac{1}{2}\left(0.85x_2^{(k-1)}+0.3x_1^{(k-1)}+1.7\right)=0.425x_2^{(k-1)}+0.15x_1^{(k-1)}+0.85, \\ x_2^{(k)} &= \tfrac{1}{6}\left(-0.85x_1^{(k)}+1.7x_3^{(k-1)}+0.9x_2^{(k-1)}-3.4\right)=-0.14167x_1^{(k)}+0.28333x_3^{(k-1)}+0.15x_2^{(k-1)}-0.56667, \\ x_3^{(k)} &= \tfrac{1}{8}\left(-3.4x_1^{(k)}+2.55x_2^{(k)}+1.2x_3^{(k-1)}+4.25\right)=-0.425x_1^{(k)}+0.31875x_2^{(k)}+0.15x_3^{(k-1)}+0.53125. \end{aligned}$$

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Gauss-Seidel iteration and Successive over-relaxation (SOR)

Gauss-Seidel iteration, tolerance, ε=0.0005
Stopping criteria: $\|\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\|_\infty < \varepsilon$

k	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$\|\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\|_\infty$
0	0	0	0	
1	1	-5/6	-3/16	1
2	0.58333	-0.82639	0.023438	0.417
3	.58681	-.75665	.047852	0.0244
4	.62167	-.75433	.031289	0.0349
5	.62284	-.76004	.028566	0.0057
6	.61998	-.76047	.029832	0.00286
7	.61977	-.76002	.030111	0.00045 (STOP)
8	.61999	-.75996	.030020	0.00022

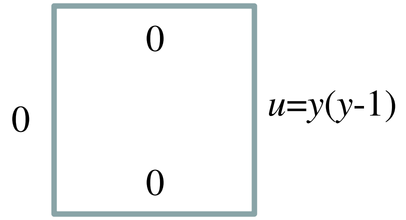
SOR iteration, tolerance, ε=0.0005
Stopping criteria: $\|\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\|_\infty < \varepsilon$

k	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$\|\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\|_\infty$
0	0	0	0	
1	.85000	-.68708	-.049008	0.85
2	.68549	-.78073	-.016291	0.1645
3	.62101	-.77637	.017408	0.064
4	.61319	-.76506	.029391	0.012
5	.61683	-.76048	.031103	0.0046
6	.61932	-.75966	.030562	0.0025
7	.62004	-.75980	.030131	0.00072
8	.62009	-.75995	.029998	0.00015 (STOP)

(ω=0.85) convergence become slow!

Partial differential equations (PDEs)

Elliptic equation : Laplace equation



E.g. Solve the Laplace equation

$$u_{xx}+u_{yy}=0,\ 0<x<1,\ 0<y<1$$

with boundary conditions

$$u(x,0) = x(x-1),\ u(x,1)=0, \qquad 0< x <1$$

$$u(0,y)=u(1,y)=0, \qquad 0\leq y \leq 1$$

using finite difference with SOR iteration, $\omega=1.25$ and $h=k=1/3$, $\mathbf{u}^{(0)}=\mathbf{0}$. All calculation in 3 DP.

Solution:

x-axis: $h=\tfrac{1}{3}$, $x_0=0$, $x_1=\tfrac{1}{3}$, $x_2=\tfrac{2}{3}$, $x_3=1$. y-axis: $k=\tfrac{1}{3}$, $y_0=0$, $y_1=\tfrac{1}{3}$, $y_2=\tfrac{2}{3}$, $y_3=1$.

Given $u(x,0)=x(x-1)$, $0\leq y \leq 1$, we get

$u_{0,0}=u(0,0)=0$; $u_{1,0}=u(\tfrac{1}{3},0)=\tfrac{1}{3}(-\tfrac{2}{3})= -0.222$; $u_{2,0}=u(\tfrac{2}{3},0)= -0.222$; $u_{3,0}=u(1,0)=0$.

Given $u(x,1)=0$, $0\leq x \leq 1$, we get

$u_{0,3}=u(0,1)=0$; $u_{1,3}=u(\tfrac{1}{3},1)=0$; $u_{2,3}=u(\tfrac{2}{3},1)=0$; $u_{3,3}=u(1,1)=0$.

Given $u(0,y)=u(1,y)=0$, $0\leq y \leq 1$, we get

$u_{0,0}=u(0,0)=0$; $u_{0,1}=u(0,\tfrac{1}{3})=0$;

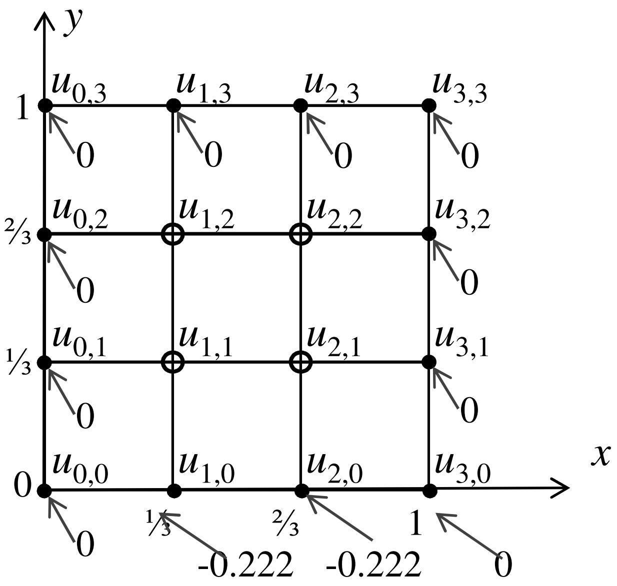
$u_{0,2}=u(0,\tfrac{2}{3})=0$; $u_{0,3}=u(0,1)=0$;

$u_{3,0}=u(1,0)=0$; $u_{3,1}=u(1,\tfrac{1}{3})=0$;

$u_{3,2}=u(1,\tfrac{2}{3})=0$; $u_{3,3}=u(1,1)=0$.

((boundary conditions symmetry on $x=\tfrac{1}{2}$))

We need to calculate for $\boldsymbol{u_{1,1}}$, $\boldsymbol{u_{2,1}}$, $\boldsymbol{u_{1,2}}$ and $\boldsymbol{u_{2,2}}$ **only**.

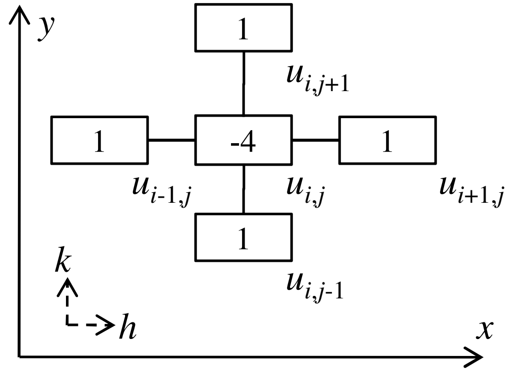


Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Using finite difference, at point (x_i,y_i), we get

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} + \left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = 0 \quad \rightarrow \quad \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = 0$$



Computational grid - implicit

Let h=k, we get

$$\boxed{u_{i,j-1} + u_{i-1,j} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1} = 0}$$

at i=1, j=1;

$u_{1,0}+u_{0,1} - 4u_{1,1} + u_{2,1} + u_{1,2}=0$
$-0.222+0 - 4u_{1,1} + u_{2,1} + u_{1,2}=0$
$- 4u_{1,1} + u_{2,1} + u_{1,2}=0.222$

at i=2, j=1;

$u_{2,0}+u_{1,1} - 4u_{2,1} + u_{3,1} + u_{2,2}=0$
$-0.222+u_{1,1} - 4u_{2,1} + 0 + u_{2,2}=0$
$u_{1,1} - 4u_{2,1} + u_{2,2}=0.222$

at i=1, j=2;

$u_{1,1}+u_{0,2} - 4u_{1,2} + u_{2,2} + u_{1,3}=0$
$u_{1,1}+0 - 4u_{1,2} + u_{2,2} + 0 =0$
$u_{1,1} - 4u_{1,2} + u_{2,2} =0$

at i=2, j=2;

$u_{2,1}+u_{1,2} - 4u_{2,2} + u_{3,2} + u_{2,3}=0$
$u_{2,1}+u_{1,2} - 4u_{2,2} + 0 + 0 =0$
$u_{2,1}+u_{1,2} - 4u_{2,2} =0$

$$\mathbf{Au} = \mathbf{b} \quad \rightarrow \quad \begin{bmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{bmatrix} \cdot \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ u_{1,2} \\ u_{2,2} \end{bmatrix} = \begin{bmatrix} 0.222 \\ 0.222 \\ 0 \\ 0 \end{bmatrix}$$

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Gauss-Seidel method: $\boxed{(\mathbf{D}+\mathbf{L}_s)\mathbf{x}^{(k)}= -\mathbf{U}_s\mathbf{x}^{(k\text{-}1)}+\mathbf{b}}$ **SOR method**: $\boxed{(\mathbf{D}+\omega\mathbf{L}_s)\mathbf{x}^{(k)}= -\ \omega\mathbf{U}_s\mathbf{x}^{(k\text{-}1)}+\omega\mathbf{b}+(1\text{-}\omega)\mathbf{D}\mathbf{x}^{(k\text{-}1)}}$

E.g. solve the below system with initial value $\mathbf{x}^{(0)}=(0,0,0)^T$ using Gauss-Seidel method and SOR (ω=1.25).

$$\mathbf{Au}=\mathbf{b} \rightarrow \begin{bmatrix}-4 & 1 & 1 & 0\\ 1 & -4 & 0 & 1\\ 1 & 0 & -4 & 1\\ 0 & 1 & 1 & -4\end{bmatrix}\cdot\begin{bmatrix}u_{1,1}\\ u_{2,1}\\ u_{1,2}\\ u_{2,2}\end{bmatrix}=\begin{bmatrix}0.222\\ 0.222\\ 0\\ 0\end{bmatrix}$$

So, we get $\mathbf{D}=\begin{bmatrix}-4 & 0 & 0 & 0\\ 0 & -4 & 0 & 0\\ 0 & 0 & -4 & 0\\ 0 & 0 & 0 & -4\end{bmatrix}$, $\mathbf{L}_s=\begin{bmatrix}0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 1 & 1 & 0\end{bmatrix}$, $\mathbf{U}_s=\begin{bmatrix}0 & 1 & 1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}$ $\rightarrow \mathbf{A}=\mathbf{D}+\mathbf{L}_s+\mathbf{U}_s$

G-S:

$$\begin{bmatrix}-4 & 0 & 0 & 0\\ 1 & -4 & 0 & 0\\ 1 & 0 & -4 & 0\\ 0 & 1 & 1 & -4\end{bmatrix}\mathbf{u}^{(k)}=-\begin{bmatrix}0 & 1 & 1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}\mathbf{u}^{(k-1)}+\begin{bmatrix}0.222\\ 0.222\\ 0\\ 0\end{bmatrix} \rightarrow$$

$$\boxed{\begin{aligned}
u_{1,1}^{(k)} &= -\tfrac{1}{4}\left(-u_{2,1}^{(k-1)}-u_{1,2}^{(k-1)}+0.222\right)=\left(+u_{2,1}^{(k-1)}+u_{1,2}^{(k-1)}-0.222\right)/4\\
u_{2,1}^{(k)} &= -\tfrac{1}{4}\left(-u_{1,1}^{(k)}-u_{2,2}^{(k-1)}+0.222\right)=\left(+u_{1,1}^{(k)}+u_{2,2}^{(k-1)}-0.222\right)/4\\
u_{1,2}^{(k)} &= -\tfrac{1}{4}\left(-u_{1,1}^{(k)}-u_{2,2}^{(k-1)}\right)=0.25u_{1,1}^{(k)}+0.25u_{2,2}^{(k)}\\
u_{2,2}^{(k)} &= -\tfrac{1}{4}\left(-u_{2,1}^{(k)}-u_{1,2}^{(k)}\right)=0.25u_{2,1}^{(k)}+0.25u_{1,2}^{(k)}
\end{aligned}}$$

SOR:

$$\begin{bmatrix}-4 & 0 & 0 & 0\\ 1.25(1) & -4 & 0 & 0\\ 1.25(1) & 0 & -4 & 0\\ 0 & 1.25(1) & 1.25(1) & -4\end{bmatrix}\mathbf{u}^{(k)}=-1.25\begin{bmatrix}0 & 1 & 1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}\mathbf{u}^{(k-1)}+1.25\begin{bmatrix}0.222\\ 0.222\\ 0\\ 0\end{bmatrix}-0.25\begin{bmatrix}-4 & 0 & 0 & 0\\ 0 & -4 & 0 & 0\\ 0 & 0 & -4 & 0\\ 0 & 0 & 0 & -4\end{bmatrix}\mathbf{u}^{(k-1)}$$

$$\rightarrow \boxed{\begin{aligned}
u_{1,1}^{(k)} &= -\tfrac{1}{4}\left(-1.25u_{2,1}^{(k-1)}-1.25u_{1,2}^{(k-1)}+u_{1,1}^{(k-1)}+0.2775\right)=\left(+1.25u_{2,1}^{(k-1)}+1.25u_{1,2}^{(k-1)}-u_{1,1}^{(k-1)}-0.2775\right)/4\\
u_{2,1}^{(k)} &= -\tfrac{1}{4}\left(-1.25u_{1,1}^{(k)}-1.25u_{2,2}^{(k-1)}+u_{2,1}^{(k-1)}+0.2775\right)=\left(+1.25u_{1,1}^{(k)}+1.25u_{2,2}^{(k-1)}-u_{2,1}^{(k-1)}-0.2775\right)/4\\
u_{1,2}^{(k)} &= -\tfrac{1}{4}\left(-1.25u_{1,1}^{(k)}-1.25u_{2,2}^{(k-1)}+u_{1,2}^{(k-1)}\right)=\left(+1.25u_{1,1}^{(k)}+1.25u_{2,2}^{(k-1)}-u_{1,2}^{(k-1)}\right)/4\\
u_{2,2}^{(k)} &= -\tfrac{1}{4}\left(-1.25u_{2,1}^{(k)}-1.25u_{1,2}^{(k)}+u_{2,2}^{(k-1)}\right)=\left(+1.25u_{2,1}^{(k)}+1.25u_{1,2}^{(k)}-u_{2,2}^{(k-1)}\right)/4
\end{aligned}}$$

Partial differential equations (PDEs)

Elliptic equation : Laplace equation

Gauss-Seidel iteration, tolerance, $\varepsilon=0.001$
Stopping criteria: $\|\mathbf{u}^{(k)}-\mathbf{u}^{(k-1)}\|_\infty < \varepsilon$

k	$u_{1,1}^{(k)}$	$u_{2,1}^{(k)}$	$u_{1,2}^{(k)}$	$u_{2,2}^{(k)}$	$\|\mathbf{u}^{(k)}-\mathbf{u}^{(k-1)}\|_\infty$
0	0	0	0	0	
1	-.056	-.069	-.014	-.021	0.069
2	-.076	-.080	-.024	-.026	0.020
3	-.082	-.082	-.027	-.027	0.006
4	-0.083	-0.083	-0.027	-0.028	0.001
5	-0.083	-0.083	-0.028	-0.028	0.001
6	-0.083	-0.083	-0.028	-0.028	0.000 (STOP)

SOR iteration, tolerance, $\varepsilon=0.001$
Stopping criteria: $\|\mathbf{u}^{(k)}-\mathbf{u}^{(k-1)}\|_\infty < \varepsilon$

k	$u_{1,1}^{(k)}$	$u_{2,1}^{(k)}$	$u_{1,2}^{(k)}$	$u_{2,2}^{(k)}$	$\|\mathbf{u}^{(k)}-\mathbf{u}^{(k-1)}\|_\infty$
0	0	0	0	0	
1	-.069	-.091	-.022	-.035	0.091
2	-.087	-.085	-.033	-.028	0.018
3	-.085	-.083	-.027	-.027	0.006
4	-.083	-.083	-.028	-.028	0.003
5	-.083	-.083	-.028	-.028	0.000 (STOP)

The solutions are: (symmetry on $x=½$)

$u(⅓, ⅓)\approx u_{1,1}=$ -0.083; $u(⅔,⅓)\approx u_{2,1}=$ -0.083;
$u(⅓, ⅔)\approx u_{1,2}=$ -0.028; $u(⅔, ⅔)\approx u_{2,2}=$ -0.028;

3 D.P.: We use $\varepsilon=0.005$, accurate up to 2 decimal places.

Partial differential equations (PDEs)

Laplace equation – simple irregular boundary

E.g. Solve the Laplace equation (Heat equation)

$$T_{xx}+T_{yy}=0,$$

with irregular boundary conditions given.

$\Delta x=h=\Delta y=k$, $\alpha_2=\beta_2=1$, $\alpha_1=\beta_1=0.7$. Solve using finite difference with Gauss-Siedel iteration.

$\mathbf{T}^{(0)}=(50,50,50,50)^T$. All calculation in 3 DP.

Solution:

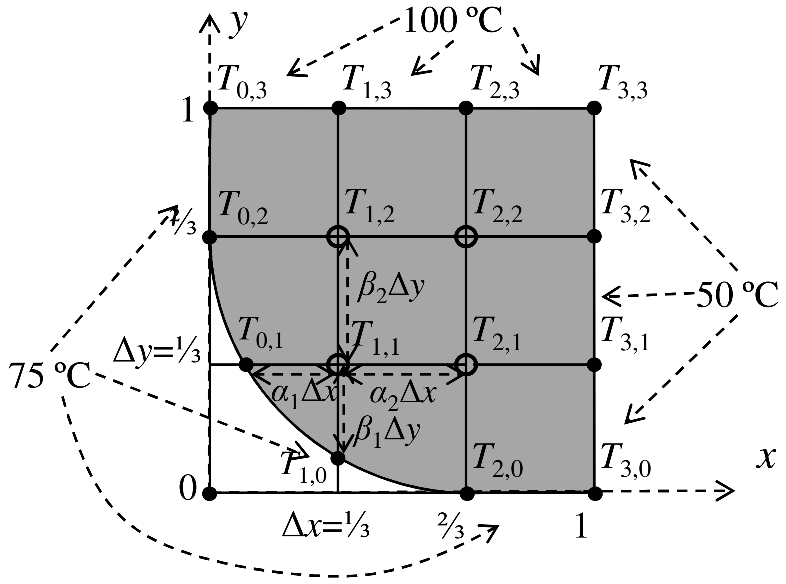
We need to calculate for $\mathbf{T_{1,1}}$, $\mathbf{T_{2,1}}$, $\mathbf{T_{1,2}}$ and $\mathbf{T_{2,2}}$ **only**.

Numerical derivative of unequally spaced data can be calculated using Lagrange interpolation.

The n-order Lagrange interpolation is given:

$$f(x)=f_n(x)+\frac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!}f^{(n+1)}(\xi(x)),\quad x_0<\xi<x_n$$

$$where\ \ f_n(x)=\sum_{i=0}^{n}L_i(x)f(x_i),\quad L_i(x)=\prod_{\substack{j=0\\ j\neq i}}^{n}\frac{x-x_j}{x_i-x_j}.$$



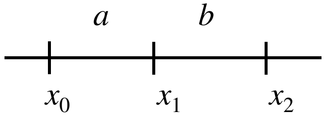
The 2-order Lagrange interpolation, with $x_0<x<x_2$, we get

$$f(x)=f(x)+O((x-x_0)(x-x_1)(x-x_2))\quad\rightarrow$$

$$f(x)=\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

or

$$f(x)=\frac{(x-x_1)(x-x_2)}{a(a+b)}f(x_0)-\frac{(x-x_0)(x-x_2)}{ab}f(x_1)+\frac{(x-x_0)(x-x_1)}{b(a+b)}f(x_2)$$



Then

We get

$$\frac{d}{dx}f(x)=f'(x)=f'(x)+O'((x-x_0)(x-x_1)(x-x_2)),$$

$$\frac{d^2}{dx^2}f(x)=f''(x)=f''(x)+O''((x-x_0)(x-x_1)(x-x_2)).$$

Partial differential equations (PDEs)

Laplace equation – simple irregular boundary

We get

$$f'(x) = \frac{f(x_0)}{a(a+b)}[2x - x_1 - x_2] - \frac{f(x_1)}{ab}[2x - x_0 - x_2] + \frac{f(x_2)}{b(a+b)}[2x - x_0 - x_1]$$

and

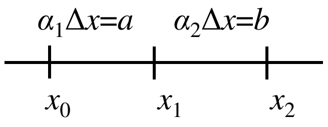
$$f''(x) = \boxed{\frac{f(x_0)}{a(a+b)}2 - \frac{f(x_1)}{ab}2 + \frac{f(x_2)}{b(a+b)}2} = \frac{2}{a(a+b)}[f(x_0) - f(x_1)] + \frac{2}{b(a+b)}[f(x_2) - f(x_1)],$$

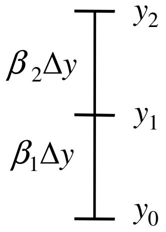
$$O' = O\left(\sum\nolimits_{i \neq j} (x - x_i)(x - x_j)\right)$$

$$\rightarrow \quad O' = O\left(\max_{i \neq j} (x - x_i)(x - x_j)\right) \approx O\left((\Delta x)^2\right)$$

$$O'' = O\left(\sum\nolimits_i 2(x - x_i)\right) = O\left(\max_i (x - x_i)\right) \approx O(\Delta x)$$

Now, change the variable for $f \rightarrow T$, $a \rightarrow \alpha_1 \Delta x$, $b \rightarrow \alpha_2 \Delta x$, we get the below results for $x_{i-1} < x < x_{i+1}$ (it is same for y-axis).





$$\frac{\partial^2 T}{\partial x^2} = \frac{2}{\Delta x^2}\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)}\right], \quad \frac{\partial^2 T}{\partial y^2} = \frac{2}{\Delta y^2}\left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)}\right]$$

Finally, the Laplace equation is given

$$\frac{2}{\Delta x^2}\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)}\right] + \frac{2}{\Delta y^2}\left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)}\right] = 0$$

If $\Delta x = \Delta y$, we get

$$\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)}\right] + \left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)}\right] = 0$$

$$\rightarrow \boxed{(\beta_1 + \beta_2)\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2}\right] + (\alpha_1 + \alpha_2)\left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2}\right] = 0}$$

Given $\alpha_1 = \beta_1 = 0.7$, $\alpha_2 = \beta_2 = 1$, we get

$$^{1.7}\!/_{0.7}\left(T_{i-1,j} - T_{i,j}\right) + 1.7\left(T_{i+1,j} - T_{i,j}\right) + {}^{1.7}\!/_{0.7}\left(T_{i,j-1} - T_{i,j}\right) + 1.7\left(T_{i,j+1} - T_{i,j}\right) = 0 \quad \rightarrow \quad \boxed{^{1.7}\!/_{0.7} T_{i,j-1} + {}^{1.7}\!/_{0.7} T_{i-1,j} - {}^{289}\!/_{35} T_{i,j} + 1.7 T_{i+1,j} + 1.7 T_{i,j+1} = 0}$$

Big Oh properties:

- Let k=constant, then $O(k \times g) = O(g)$; if $f = O(g)$ then $k \times f = O(g)$
- If $f(n) = O(g(n))$ and $g(n) = O(h(n))$ then $f(n) = O(h(n))$
- If $f_1(n) = O(g_1(n))$, $f_2(n) = O(g_2(n))$, then $f_1(n) \times f_2(n) = \mathrm{O}(g_1(n) \times g_2(n))$
- If $f_1(n) = O(g_1(n))$ and $f_2(n) = O(g_2(n))$ then $f_1(n) + f_2(n) = O(\max[g_1, g_2])$

Partial differential equations (PDEs)

Laplace equation – simple irregular boundary

Node i=1, j=1 $\boxed{{}^{1.7}\!/_{0.7}T_{i,j-1} + {}^{1.7}\!/_{0.7}T_{i-1,j} - {}^{289}\!/_{35}T_{i,j} + 1.7T_{i+1,j} + 1.7T_{i,j+1} = 0}$

$$\boxed{T_{i,j-1} + T_{i-1,j} - 4T_{i,j} + T_{i+1,j} + T_{i,j+1} = 0}$$

For nodes (i, j)=(2,1), (1,2) & (2,2).

At i=1, j=1; (irregular node)

$(1.7/0.7)T_{0,1}+1.7T_{2,1} +(1.7/0.7)T_{1,0}+1.7T_{1,2}-(289/35)T_{1,1}=0$

$(1.7/0.7)75+1.7T_{2,1} +(1.7/0.7)75+1.7T_{1,2}-(289/35)T_{1,1}=0$

$-(289/35)T_{1,1}+1.7T_{2,1} +1.7T_{1,2}= -364.286$

At i=2, j=1; (normal computational node)

$T_{2,0} + T_{1,1} - 4T_{2,1} + T_{3,1} +T_{2,2} = 0$

$75 + T_{1,1} - 4T_{2,1} + 50 +T_{2,2} = 0$

$T_{1,1} - 4T_{2,1} +T_{2,2} = -125$

At i=1, j=2; (normal computational node)

$T_{1,1}+ T_{0,2} - 4T_{1,2} + T_{2,2} + T_{1,3}=0$

$T_{1,1}+ 75 - 4T_{1,2} + T_{2,2} + 100 = 0$

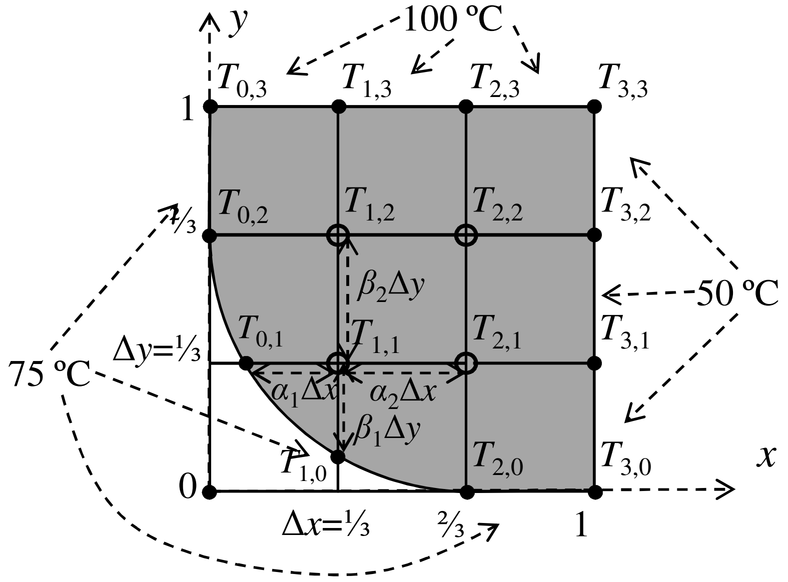
$T_{1,1} - 4T_{1,2} + T_{2,2} = - 175$

At i=2, j=2; (normal computational node)

$T_{2,1}+ T_{1,2}- 4T_{2,2} + T_{3,2} + T_{2,3}=0$

$T_{2,1}+ T_{1,2}- 4T_{2,2} + 50 + 100 = 0$

$T_{2,1}+ T_{1,2}- 4T_{2,2} = - 150$



$$\mathbf{AT} = \mathbf{b} \rightarrow \begin{bmatrix} -{}^{289}\!/_{35} & 1.7 & 1.7 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{bmatrix} \cdot \begin{bmatrix} T_{1,1} \\ T_{2,1} \\ T_{1,2} \\ T_{2,2} \end{bmatrix} = \begin{bmatrix} -364.286 \\ -125 \\ -175 \\ -150 \end{bmatrix}$$

Partial differential equations (PDEs)

Laplace equation – simple irregular boundary

Gauss-Seidel method: $\boxed{(\mathbf{D}+\mathbf{L}_s)\mathbf{x}^{(k)} = -\mathbf{U}_s\mathbf{x}^{(k\text{-}1)}+\mathbf{b}}$

E.g. solve the below system with initial value $\mathbf{T}^{(0)}=(50,50,50,50)^T$ using Gauss-Seidel method.

$$\mathbf{AT}=\mathbf{b} \rightarrow \begin{bmatrix} -{}^{289}\!/_{35} & 1.7 & 1.7 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{bmatrix} \cdot \begin{bmatrix} T_{1,1} \\ T_{2,1} \\ T_{1,2} \\ T_{2,2} \end{bmatrix} = \begin{bmatrix} -364.286 \\ -125 \\ -175 \\ -150 \end{bmatrix}$$

So, we get

$$\begin{aligned} T_{1,1}^{(k)} &= -{}^{35}\!/_{289}\left(-1.7T_{2,1}^{(k-1)} - 1.7T_{1,2}^{(k-1)} - 364.286\right) \\ T_{2,1}^{(k)} &= -{}^{1}\!/_{4}\left(-T_{1,1}^{(k)} - T_{2,2}^{(k-1)} - 125\right) \\ T_{1,2}^{(k)} &= -{}^{1}\!/_{4}\left(-T_{1,1}^{(k)} - T_{2,2}^{(k-1)} - 175\right) \\ T_{2,2}^{(k)} &= -{}^{1}\!/_{4}\left(-T_{2,1}^{(k)} - T_{1,2}^{(k)} - 150\right) \end{aligned}$$

Gauss-Seidel iteration, tolerance, $\varepsilon=0.001$

Stopping criteria: $\|\mathbf{T}^{(k)}-\mathbf{T}^{(k\text{-}1)}\|_\infty < \varepsilon$

k	$T_{1,1}^{(k)}$	$T_{2,1}^{(k)}$	$T_{1,2}^{(k)}$	$T_{2,2}^{(k)}$	$\|\mathbf{T}^{(k)}-\mathbf{T}^{(k\text{-}1)}\|_\infty$
0	50	50	50	50	
1	64.706	59.926	72.426	70.588	22.4
2	71.367	66.739	79.239	73.994	6.8
3	74.172	68.291	80.791	74.771	2.8
4	74.811	68.646	81.146	74.948	0.639
5	74.957	68.726	81.226	74.988	0.146
6	74.990	68.745	81.245	74.997	0.033
7	74.998	68.749	81.249	74.999	0.008
8	75.000	68.750	81.250	75.000	0.002
9	75.000	68.750	81.250	75.000	0.000 (Stop)

The solutions are: (no symmetry property)

$T(⅓, ⅓)\approx T_{1,1}=$ 75.000; $T(⅔,⅓)\approx T_{2,1}=$ 68.750;
$T(⅓, ⅔)\approx T_{1,2}=$ 81.250; $T(⅔, ⅔)\approx T_{2,2}=$ 75.000;

Partial differential equations (PDEs)

Parabolic equation

Heat conduction equation is given

$u_t = c^2 u_{xx}$, or $\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}$ $0 < x < a,\ t > 0$

with boundary conditions

$pu_x(0,t) + ru(0,t) = g_1(t), \quad t > 0$

$qu_x(a,t) + su(a,t) = g_2(t), \quad t > 0$

and initial condition

$u(x,0) = f(x), \quad 0 \le x \le a.$

If $p=q=0$, it is named as **Dirichlet problem**. If $r=s=0$, it is called **Neumann problem**. The other Conditions is called as **Robin b.c.** (**mixed b.c.**). Currently, we will study on Dirichlet problem as below:

$u(0,t) = g_1(t) = c_1, \quad t \ge 0,$

$u(a,t) = g_2(t) = c_2, \quad t \ge 0.$

$$f'(x_i) = \frac{1}{h}[f(x_{i+1}) - f(x_i)] - \frac{h}{2} f^{(2)}(\xi_i),\ x_i < \xi_i < x_{i+1}.$$

Forward difference method

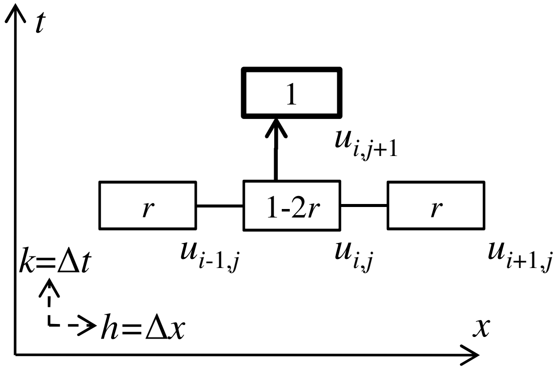
At point (x_i, t_j), we get

Let $r = c^2k/h^2$, we get

$$\left(\frac{\partial u}{\partial t}\right)_{i,j} = c^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \rightarrow \frac{u_{i,j+1} - u_{i,j}}{k} = c^2 \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}$$

$$\rightarrow \quad u_{i,j+1} - u_{i,j} = c^2 \frac{k}{h^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)$$

$$\boxed{u_{i,j+1} = ru_{i-1,j} + (1-2r)u_{i,j} + ru_{i+1,j}}$$ → Explicit method



Computational grid - explicit

Stability condition: $r = c^2k/h^2 \le ½$.

(note: let c=1, this method very slow. If $\Delta x = h = 0.01$, then $\Delta t = k \le 5 \times 10^{-5}$,very slow)

Partial differential equations (PDEs)

Parabolic equation

E.g. solve the heat conduction equation

$u_t=u_{xx}$, $0< x <1$, $t >0$

with boundary conditions

$u(0,t) = u(1,t) = 0$, $t >0$

and initial value condition

$u(x,0) = x(1-x)$, $0\leq x \leq 1$.

Using explicit finite difference method (or forward difference method) with $h=\Delta x=1/5$, $k=\Delta t=1/100$, find the solution up to $t=0.02$. All calculation in 3 DP. Analytical solution is given: $u(x,t) = {}^{8}\!/_{\pi^3} \sum_{i=1,3,\cdots}^{\infty} {}^{1}\!/_{r^3} \exp\left(-r^2\pi t\right)\sin\left(i\pi x\right)$

Solution:

x-axis: $h=1/5$, $x_0=0$, $x_1=0.2$, $x_2=0.4$, $x_3=0.6$, $x_4=0.8$, $x_5=1$.

y-axis: $k=1/100$, $t_0=0$, $t_1=0.01$, $t_2=0.02$.

Given $u(0,t) = u(1,t) = 0$, $t >0$, so

$u_{0,1}=u(0,0.01)=0$, $u_{0,2} =u(0,0.02)=0$,

$u_{5,1}=u(1,0.01)=0$, $u_{5,2}=u(1,0.02)=0$.

Given $u(x,0) = x(1-x)$, $0\leq x\leq 1$, we get

$u_{0,0}=u(0,0)=0(1-0) =0$, $u_{1,0}=u(0.2,0)=0.2(1-0.2) =0.160$,

$u_{2,0}=u(0.4,0)=0.4(1-0.4) =0.240$,

$u_{3,0}=u(0.6,0)=0.6(1-0.6) =0.240$,

$u_{4,0}=u(0.8,0)=0.8(1-0.8) =0.160$,

$u_{5,0}=u(1.0,0)=1.0(1-1.0) =0$.

So, we only need to calculate for $u_{1,1}$, $u_{2,1}$, $u_{3,1}$, $u_{4,1}$, $u_{1,2}$, $u_{2,2}$, $u_{3,2}$, and $u_{4,2}$.

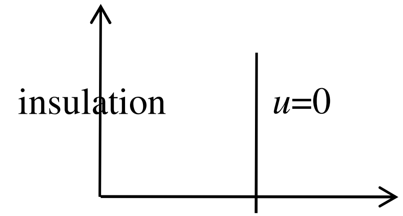
(note: initial value condition show that solutions are symmetry at x=½)

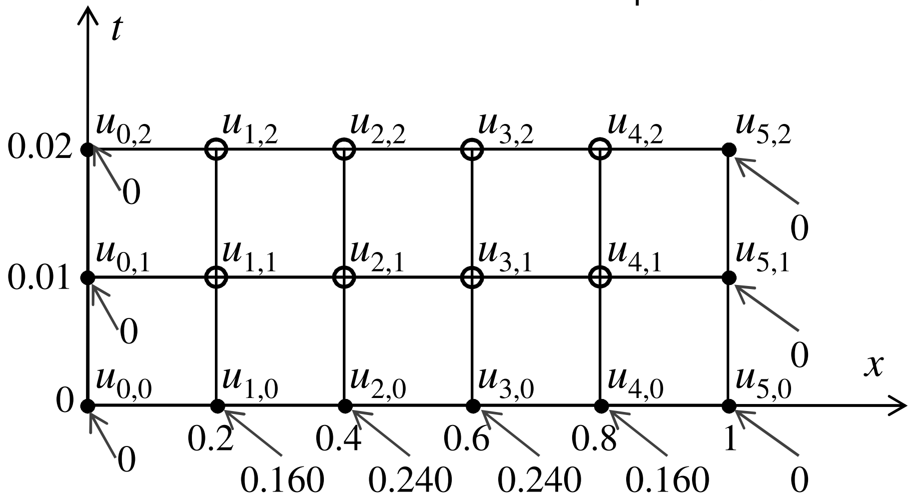
Let $X=a-x$

$$\frac{\partial u}{\partial x}=\frac{\partial u}{\partial X}\frac{dX}{dx}=-\frac{\partial}{\partial X}u \quad\rightarrow\quad \frac{\partial}{\partial x}=-\frac{\partial}{\partial X},\rightarrow\frac{\partial^2}{\partial x^2}=\frac{\partial^2}{\partial X^2}$$

$$u_t=u_{xx} \quad\leftrightarrow\quad u_t=u_{XX}$$

So, $u(x,y)$ is symmetry on $x=a$!





Partial differential equations (PDEs)

Parabolic equation

At point (x_i,t_j), we get $\left(\frac{\partial u}{\partial t}\right)_{i,j} = \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \to \frac{u_{i,j+1}-u_{i,j}}{k} = \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2} \to u_{i,j+1}-u_{i,j} = \frac{k}{h^2}\left(u_{i+1,j}-2u_{i,j}+u_{i-1,j}\right)$

Let $r = k/h^2$, we get $u_{i,j+1} = ru_{i-1,j} + (1-2r)u_{i,j} + ru_{i+1,j} \quad (r = {}^{k}\!/_{h^2} = {}^{1/100}\!/_{1/5^2} = {}^{1}\!/_{4}) \to \boxed{u_{i,j+1} = {}^{1}\!/_{4}u_{i-1,j} + {}^{1}\!/_{2}u_{i,j} + {}^{1}\!/_{4}u_{i+1,j}}$

At j=0, we get

$u_{1,1}$=¼($u_{0,0}$+2$u_{1,0}$+$u_{2,0}$)=¼[0+2(0.160)+0.240]=0.140,
$u_{2,1}$=¼($u_{1,0}$+2$u_{2,0}$+$u_{3,0}$)=¼[0.160+2(0.240)+0.240]=0.220,
$u_{3,1}$=¼($u_{2,0}$+2$u_{3,0}$+$u_{4,0}$)=¼[0.240+2(0.240)+0.160]=0.220,
$u_{4,1}$=¼($u_{3,0}$+2$u_{4,0}$+$u_{5,0}$)=¼[0.240+2(0.160)+0]=0.140.

At j=1, we get

$u_{1,2}$=¼($u_{0,1}$+2$u_{1,1}$+$u_{2,1}$)=¼[0+2(0.140)+0.220]=0.125,
$u_{2,2}$=¼($u_{1,1}$+2$u_{2,1}$+$u_{3,1}$)=¼[0.140+2(0.220)+0.220]=0.200,
$u_{3,2}$=¼($u_{2,1}$+2$u_{3,1}$+$u_{4,1}$)=¼[0.220+2(0.220)+0.140]=0.200,
$u_{4,2}$=¼($u_{3,1}$+2$u_{4,1}$+$u_{5,1}$)=¼[0.220+2(0.140)+0]=0.125.

The solutions are: (symmetry on x= ½)

u(0.2,0.01)≈$u_{1,1}$=0.140; u(0.4,0.01)≈$u_{2,1}$=0.220;
u(0.6,0.01)≈$u_{3,1}$=0.220; u(0.8,0.01)≈$u_{4,1}$=0.140;
u(0.2,0.02)≈$u_{1,2}$=0.125; u(0.4,0.02)≈$u_{2,2}$=0.200;
u(0.6,0.02)≈$u_{3,2}$=0.200; u(0.8,0.02)≈$u_{4,2}$=0.125;

The accuracy can be increased by using the below numerical integration:

Centered-difference formula:

$$\boxed{f'(x_i) = \frac{1}{2h}\left[f(x_{i+1}) - f(x_{i-1})\right] - \frac{h^2}{6} f^{(3)}(\xi_i), \quad x_{i-1} < \xi_i < x_{i+1}.}$$

2nd order forward difference (or 3-point formula):

$$\boxed{f'(x_i) = \frac{1}{2h}\left[-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})\right] + \frac{h^2}{3} f^{(3)}(\xi_i),\ x_i < \xi_i < x_{i+2}.}$$

2nd order backward difference (or 3-point formula):

$$\boxed{f'(x_i) = \frac{1}{2h}\left[3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})\right] + \frac{h^2}{3} f^{(3)}(\xi_i),\ x_{i-2} < \xi_i < x_i.}$$

Partial differential equations (PDEs)

Parabolic equation : implicit Crank-Nicolson method

Implicit method

At point $(x_i, t_{j+½})$, we get

$$\left(\frac{\partial u}{\partial t}\right)_{i,j+½} = c^2\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j+½} \rightarrow \left(\frac{\partial u}{\partial t}\right)_{i,j+½} = c^2\ ½\left(\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j+1} + \left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j}\right)$$

$$\rightarrow \frac{u_{i,j+1} - u_{i,j}}{2\left(k/2\right)} = c^2\ ½\left(\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}\right)$$

Finally, we get

$2(u_{i,j+1} - u_{i,j}) = c^2k/h^2\ (u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1} + u_{i+1,j} - 2u_{i,j} + u_{i-1,j})$

Now, let $r = c^2k/h^2$, we get

$$\boxed{-\ ru_{i-1,j+1} + (2+2r)\ u_{i,j+1} - ru_{i+1,j+1} = r\ u_{i-1,j} + (2-2r)\ u_{i,j} + ru_{i+1,j}}$$

with computational grid for r=1 and r =any value.

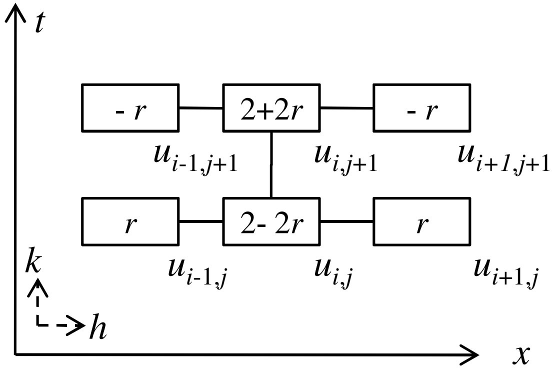
The Crank-Nicolson method will produce linear system

Au=b

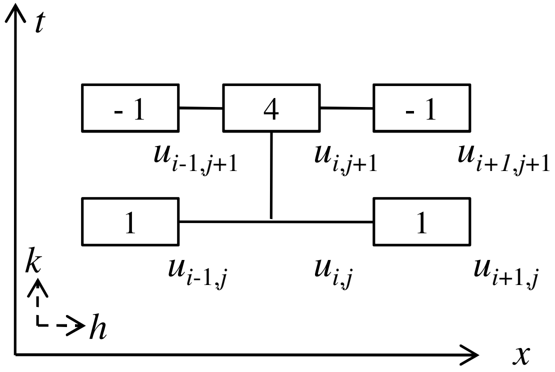
With **A** is tridiagonal matrix. So, the linear system can be solved using Thomas algorithm. Since the matrix **A** is also diagonally dominant, so iteration method can be applied e.g. Gauss-Seidel iteration technique.

Crank-Nicolson method is stable for any value of r.

However, smaller value of h=Δx, k= Δt are required for higher accuracy.



Computational grid - implicit



Computational grid – implicit (r=1)

Partial differential equations (PDEs)

Parabolic equation : implicit Crank-Nicolson method

E.g. solve the heat conduction equation

$u_t = u_{xx}$, $\quad 0 < x < 1,\ t > 0$

with boundary conditions

$u(0,t) = u(1,t) = 0$, $\quad t > 0$

and initial value condition

$$u(x,0) = \begin{cases} 2x, & 0 \le x \le \frac{1}{2} \\ 2(1-x), & \frac{1}{2} \le x \le 1 \end{cases}$$

Using Crank-Nicolson method with $h=\Delta x=0.2$, $k=\Delta t=0.04$, find the solution at $t=0.04$ only. All calculation in 3 DP. Use Gauss-Seidel iteration to solve the linear system.

Solution:

x-axis: $h=0.2$, $x_0=0$, $x_1=0.2$, $x_2=0.4$, $x_3=0.6$, $x_4=0.8$, $x_5=1$.

y-axis: $k=0.04$, $t_0=0$, $t_1=0.04$.

Given $u(0,t) = u(1,t) = 0$, $t > 0$, so

$u_{0,1}=u(0,0.04)=0$, $u_{5,1}=u(1,0.04)=0$.

Given $u(x,0) = 2x$, $\quad 0 \le x \le ½$, we get

$u_{0,0}=u(0,0)=2(0)=0$, $u_{1,0}=u(0.2,0)=2(0.2)=0.4$,

$u_{2,0}=u(0.4,0)=2(0.4)=0.8$,

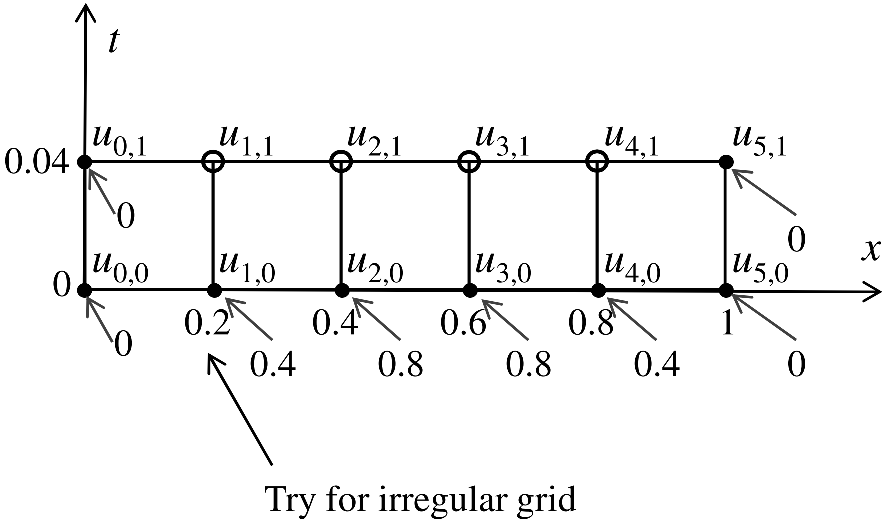
Given $u(x,0) = 2(1-x)$, $½ \le x \le 1$, we get

$u_{3,0}=u(0.6,0)=2(1-0.6)=0.8$,

$u_{4,0}=u(0.8,0)=2(1-0.8)=0.4$, $u_{5,0}=u(1.0,0)=2(1-1.0)=0$.

So, we only need to calculate for $\boldsymbol{u_{1,1}}$, $\boldsymbol{u_{2,1}}$, $\boldsymbol{u_{3,1}}$ and $\boldsymbol{u_{4,1}}$.

(note: initial value condition show that solutions are symmetry at $x=½$)



Partial differential equations (PDEs)

Parabolic equation : implicit Crank-Nicolson method

At point $(x_i, t_{j+½})$, we get $\left(\frac{\partial u}{\partial t}\right)_{i,j+½} = ½\left(\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j+1} + \left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j}\right) \rightarrow \frac{u_{i,j+1} - u_{i,j}}{2(k/2)} = ½\left(\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}\right)$

Let $r = k/h^2$, we get: $-ru_{i-1,j+1} + (2+2r)\, u_{i,j+1} - ru_{i+1,j+1} = r\, u_{i-1,j} + (2-2r)\, u_{i,j} + ru_{i+1,j}$

Since $r = k/h^2, = 0.04/0.2^2 = 1$, we get

$$\boxed{- u_{i-1,j+1} + 4u_{i,j+1} - u_{i+1,j+1} = u_{i-1,j} + u_{i+1,j}}$$

For $i=1$, $j=0$;

$- u_{0,1} + 4u_{1,1} - u_{2,1} = u_{0,0} + u_{2,0}$

$0 + 4u_{1,1} - u_{2,1} = 0 + 0.8$

$4u_{1,1} - u_{2,1} = 0.8$

For $i=2$, $j=0$;

$- u_{1,1} + 4u_{2,1} - u_{3,1} = u_{1,0} + u_{3,0}$

$- u_{1,1} + 4u_{2,1} - u_{3,1} = 0.4 + 0.8 = 1.2$

For $i=3$, $j=0$;

$- u_{2,1} + 4u_{3,1} - u_{4,1} = u_{2,0} + u_{4,0}$

$- u_{2,1} + 4u_{3,1} - u_{4,1} = 0.8 + 0.4 = 1.2$

For $i=4$, $j=0$;

$- u_{3,1} + 4u_{4,1} - u_{5,1} = u_{3,0} + u_{5,0}$

$- u_{3,1} + 4u_{4,1} - 0 = 0.8 + 0$

$- u_{3,1} + 4u_{4,1} = 0.8$

$$\mathbf{Au} = \mathbf{b} \quad \rightarrow \quad \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix} \cdot \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ u_{3,1} \\ u_{4,1} \end{bmatrix} = \begin{bmatrix} 0.8 \\ 1.2 \\ 1.2 \\ 0.8 \end{bmatrix}$$

Matrix **A** is tridiagonal matrix. It is also diagonally dominant.

Partial differential equations (PDEs)

Parabolic equation : implicit Crank-Nicolson method

Gauss-Seidel method: $\boxed{(\mathbf{D}+\mathbf{L}_s)\mathbf{u}^{(k)} = -\mathbf{U}_s\mathbf{u}^{(k-1)}+\mathbf{b}}$

E.g. solve the below system with initial value $\mathbf{u}^{(0)}=(0,0,0,0)^T$ using Gauss-Seidel method.

$$\mathbf{Au}=\mathbf{b} \quad \rightarrow \quad \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix} \cdot \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ u_{3,1} \\ u_{4,1} \end{bmatrix} = \begin{bmatrix} 0.8 \\ 1.2 \\ 1.2 \\ 0.8 \end{bmatrix}$$

So, we get

$$\begin{aligned} u_{1,1}^{(k)} &= \tfrac{1}{4}\left(u_{2,1}^{(k-1)} + 0.8\right) \\ u_{2,1}^{(k)} &= \tfrac{1}{4}\left(u_{1,1}^{(k)} + u_{3,1}^{(k-1)} + 1.2\right) \\ u_{3,1}^{(k)} &= \tfrac{1}{4}\left(u_{2,1}^{(k)} + u_{4,1}^{(k-1)} + 1.2\right) \\ u_{4,1}^{(k)} &= \tfrac{1}{4}\left(u_{3,1}^{(k)} + 0.8\right) \end{aligned}$$

G-S iteration (3 D.P.), tolerance, ε=0.005

Stopping criteria: $\|\mathbf{T}^{(k)}-\mathbf{T}^{(k-1)}\|_\infty < \varepsilon$

k	$u_{1,1}^{(k)}$	$u_{2,1}^{(k)}$	$u_{3,1}^{(k)}$	$u_{4,1}^{(k)}$	$\|\mathbf{T}^{(k)}-\mathbf{T}^{(k-1)}\|_\infty$
0	0	0	0	0	
1	.200	.350	.387	.297	0.387
2	.287	.469	.491	.323	0.119
3	.317	.502	.506	.327	0.033
4	.326	.508	.509	.327	0.009
5	.327	.509	.509	.327	0.001 (stop)

The solutions are: (symmetry on x= ½)
$u(0.2,0.04)\approx u_{1,1}$=0.327; $u(0.4,0.04)\approx u_{2,1}$=0.509;
$u(0.6,0.04)\approx u_{3,1}$=0.509; $u(0.8,0.04)\approx u_{4,1}$=0.327;

We can speed up calculation by using refined initial values, $u^{(0)}=(0.2,0.2,0.2,0.2)^T$!