Numerical Methods II

SSCM 3423

Chapter 1

This chapter formulates and writes algorithms to solve initial value problems using single and multistep methods.

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Well-posed Problem

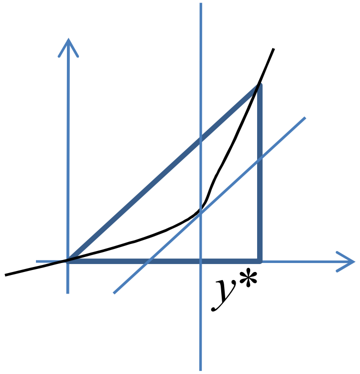
Given initial value problem (IVP)
$y'=f(x,y), \ y(a)=\eta$ (1)

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

If η is any given number, there exist a unique solution $y(x)$ where $y(x)$ is continuous and differentiable for all (x,y) in domain D and fulfill Lipschitz condition.

Using **mean value theorem**

$$f(x,y)-f(x,y^*)=\frac{\partial f(x,\bar{y})}{\partial y}(y-y^*)$$



So we choose

$$L=\sup_{(x,y)\in D}\left|\frac{\partial f(x,y)}{\partial y}\right|$$

An initial value problem that has a **unique solution** and is **stable** is called **well-posed**. If $f(t,y)$ is continuous and satisfied a **Lipschitz condition**, then the IVP is well posed.

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

Euler method

Generally, n-order ODE has the form

$$\frac{d^n y}{dt^n} = y^{(n)} = f\left(t, y, y', y'', y^{(3)}, \cdots, y^{(n-1)}\right)$$

$y'=f(t,y)$, $a \le t \le b$, $y(a)=\alpha$,

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

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

Euler method

Taylor's series at $t=a$

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

$$y(t) = y(a) + \frac{y'(a)}{1!}(t-a) + \frac{y''(a)}{2!}(t-a)^2 + \cdots + \frac{y^{(n)}(a)}{n!}(t-a)^n + R_n.$$

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

Let $y'=f$, $t_i=a$, $t_{i+1}=t$, $h=t\text{-}a$, and truncated the series after the second term, for $h \to 0$, we get

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

← Basic Euler formula, First order

Truncation error

"Big O" notation→$O(g(t))$.

Some finite value × $g(t)$

$O(h^2)$=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 $0 < M < \infty$, $\delta > 0$.

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

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

E.g. initial value problem:

$y'=y-t^2+1,\ 0 \le t \le 1,\ y(0)=0.5$ $\qquad$ $y'=f(t,y),\ a\le t\le b,\ y(a)=\alpha,$

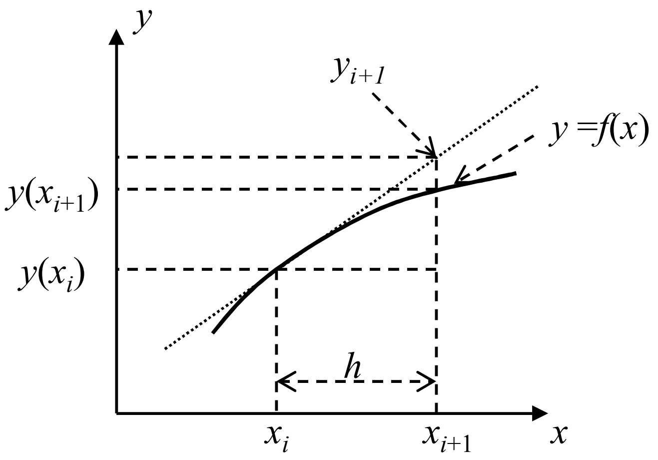
Let h =0.2, y_0=0.5, we get (here use 7 decimal places, D.P.)

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

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

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

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.

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

Taylor method – higher order one step method

Taylor's series at *t*=*a* $y'=f(t,y),\ a\le t\le b,\ y(a)=\alpha,$

$$y(t)=y(a)+\frac{y'(a)}{1!}(t-a)+\frac{y''(a)}{2!}(t-a)^2+\cdots+\frac{y^{(n)}(a)}{n!}(t-a)^n+R_n.$$

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

Let $y'=f$, $t_i=a$, $t_{i+1}=t$, $h=t-a$, and truncated the series after the second term, for $h\to 0$, we get

$$\boxed{y_{i+1}=y_i+hf(t_i,y_i)+\tfrac{1}{2}h^2\,{}^{d}\!/\!_{dt}\,f(t,y)\Big|_{t_i}+O(h^3),\quad y_{i+1}\approx y_i+hf(t_i,y_i)+\tfrac{1}{2}h^2\left({}^{\partial f}\!/\!_{\partial t}+{}^{\partial f}\!/\!_{\partial y}\,f\right)\Big|_{t_i}}$$

Second - order Taylor method

E.g. Consider IVP $\dfrac{dx}{dt}=1+\dfrac{x}{t},\quad (1\le t\le 6),\ \ x(1)=1.$

$$\Longrightarrow$$

$$f(t,y)=1+\frac{x}{t}$$

$$\frac{d}{dt}f(t,y)=\frac{tx'-x}{t^2}=\frac{x'}{t}-\frac{x}{t^2}=\frac{1}{t}\left(1+\frac{x}{t}\right)-\frac{x}{t^2}$$

$$=\frac{1}{t}$$

Exact solution: $x(t)=t(1+\ln t)$

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

Second-order Runge-Kutta Method $y'=f(t,y),\ a\le t\le b,\ y(a)=\alpha,$

Assume

$$\boxed{\frac{y(t+h)-y(t)}{h}=a_1 f(t,y)+a_2 f\big(t+\alpha_2, y+\delta_2 f(t,y)\big)}$$

Higher dimension Taylor expansion

$$f(x+a,y+b)=f(x,y)+\frac{1}{1!}D_1[f(x,y)]+\frac{1}{2!}D_2[f(x,y)]+\cdots+\frac{1}{n!}D_n[f(x,y)]+R_n.$$

$$D_n=\left(a\frac{\partial}{\partial x}+b\frac{\partial}{\partial y}\right)^n \quad R_n=\frac{1}{(n+1)!}D_{n+1}[f(x+\theta_1 a, y+\theta_2 b)]$$

$$0<\theta_1<1,\ 0<\theta_2<1.$$

We get

$$f(t+\Delta t,y+\Delta y)=f(t,y)+\left[\Delta t\frac{\partial f(t,y)}{\partial t}+\Delta y\frac{\partial f(t,y)}{\partial y}\right]$$

$$\left.+\left[\frac{(\Delta t)^2}{2}\frac{\partial^2 f(\xi,\eta)}{\partial t^2}+\Delta t\Delta y\frac{\partial^2 f(\xi,\eta)}{\partial t\partial y}++\frac{(\Delta y)^2}{2}\frac{\partial^2 f(\xi,\eta)}{\partial y^2}\right]\right\} O(\Delta t^2)$$

Second order Taylor method

$$\boxed{y(t+h)=y+hf(t,y)+\tfrac{1}{2}h^2\,{}^{d}\!/_{dt}\,f(t,y)\big|_{t_i}+O(h^3),\quad y(t+h)\approx y+hf(t,y)+\tfrac{1}{2}h^2\left({}^{\partial f}\!/_{\partial t}+{}^{\partial f}\!/_{\partial y}\,f\right)}$$

$$\frac{y(t+h)-y(t)}{h}=a_1 f(t,y)+a_2 f\big(t+\alpha_2,y+\delta_2 f(t,y)\big)$$

$$=a_1 f(t,y)+a_2\left[f(t,y)+\alpha_2\frac{\partial f}{\partial t}+\delta_2 f(t,y)\frac{\partial f}{\partial y}+R_1\right]$$

$$=(a_1+a_2)f(t,y)+a_2\alpha_2\frac{\partial f}{\partial t}+a_2\delta_2 f(t,y)\frac{\partial f}{\partial y}+a_2R_1$$

$$R_1=\left[\alpha_2^2\frac{\partial^2 f(\xi,\eta)}{\partial t^2}+\alpha_2\delta_2 f(t,y)\frac{\partial^2 f(\xi,\eta)}{\partial t\partial y}+\delta_2^2 f^2(t,y)\frac{\partial^2 f(\xi,\eta)}{\partial y^2}\right]=O(h^2)$$

$$\left.\begin{aligned} a_1+a_2&=1\\ a_2\alpha_2&=h/2\\ a_2\delta_2&=h/2 \quad \rightarrow \alpha_2=\delta_2=h/(2a_2)\end{aligned}\right.$$

3 Eqs with **4 unknown** leads to non-uniquely solution. **undetermined systems**

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

Second-order Runge-Kutta Method $y'=f(t,y),\ a\le t\le b,\ y(a)=\alpha,$

Modified Euler method
(Midpoint formulae) $a_1=0,\ a_2=1;\ \alpha_2=\delta_2=h/2$

$$y^* = y_i + \frac{h}{2} f(t_i, y_i),$$

$$y_{i+1} \approx y_i + hf(t_i + h/2, y^*).$$

Improved Euler's formula
(Heun method) $a_1=a_2=1/2\ ;\ \alpha_2=\delta_2=h$

$$y_{i+1} \approx y_i + \frac{1}{2}(K_1 + K_2)$$

$$K_1 = hf(t_i, y_i)$$

$$K_2 = hf(t_i + h, y_i + K_1)$$

Optimal RK2 method $a_1=1/4,\ a_2=3/4;\ \alpha_2=\delta_2=2h/3$

$$y_{i+1} \approx y_i + \frac{1}{4}(K_1 + 3K_2)$$

$$K_1 = hf(t_i, y_i)$$

$$K_2 = hf\left(t_i + \frac{2}{3}h, y_i + \frac{2}{3}K_1\right)$$

E.g. Consider IVP

$$\frac{dx}{dt} = 1 + \frac{x}{t}, \quad (1 \le t \le 6),\ x(1) = 1.$$

Exact solution: $x(t)=t(1+\ln t)$

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

Classical fourth-order Runge-Kutta Method (RK4) $y'=f(x,y)$, $a\leq x\leq b$, $y(a)=\alpha$,

RK4 is given

$$y(x+h)\approx y(x)+1/6[\,k_1+2k_2+2k_3+k_4]+O(h^5)$$

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

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

Second-order Runge-Kutta (RK2) method (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: $y(-0.5)=y(0)+ 1/6[k_1+2k_2+2k_3+k_4]=1+1/6 [-43.6875]=-6.28125.\rightarrow$ ε_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: $y(0.5)=y(0)+ 1/6[k1+2k2+2k3+k4]=2+1/6 [-43.6875]=3.7516995 \rightarrow$ ε_t**=-0.0048%**.

Ordinary differential equations (ODEs)

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

m-step multistep method for solving initial value problem:

$$y'=f(x,y),\ \ a\le x\le b,\ y(a)=\alpha,$$

is given

$$y_{i+1}=a_{m-1}y_i+a_{m-2}y_{i-1}+\ldots+a_0y_{i+1-m}$$
$$+h[b_mf(x_{i+1},y_{i+1})+b_{m-1}f(x_i,y_i)+\ldots+b_0f(x_{i+1-m},y_{i+1-m})].$$

for $i=m-1,m,\ldots,N-1$, where $h=(b-a)/N$, a_i and b_i are constants, and the starting values $y_0=\alpha$, $y_1=\alpha_1$, $y_2=\alpha_2$, …, $y_{m-1}=\alpha_{m-1}$.

When $b_m=0$ the method is called **explicit**, or **open**. When $b_m\neq0$ the method is called **implicit**, or **closed**, since y_{i+1} occurs on both sides.

Adams-Bashforth – open formulas

$$\boxed{f_i=f(x_i,y_i)}$$

Taylor series expansion around x_i

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

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

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

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

Ordinary differential equations (ODEs)

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

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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}

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

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

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

$$y_i = y(x_i + h - h) = y(x_i + h) - hy'_i + \frac{h^2}{2!}y''_i - \cdots$$

$$y^{(0)}_{i+1} \approx y_i + \frac{h}{2}\left(3f_i - f_{i-1}\right)$$

$$y^{(k+1)}_{i+1} \approx y_i + \frac{h}{2}\left(f^{(k)}_{i+1} + f_i\right)$$

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

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 $y_1^1, y_1^2, \ldots, y_1^m$. ($m$ iteration); get $y_2^1, y_2^2, \ldots, y_2^m$. ($m$ 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 Taylor series.

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

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

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

Predictor:

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

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

Second order Adams-Moulton formula

$$y^{(0)}{}_{i+1} \approx y_i + \frac{h}{2}\left(3f_i - f_{i-1}\right)$$

$$y^{(k+1)}{}_{i+1} \approx y_i + \frac{h}{2}\left(f^{(k)}{}_{i+1} + f_i\right)$$

True percent relative error, ε_t =(true value-approx)/(true value) × 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

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

Ordinary differential equations (ODEs)

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

Improved Euler method – Heun's method (Predictor-corrector method)

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

$$y'_i = f(t_i, y_i) \rightarrow \quad y^0_{i+1} = y_i + hf(t_i, y_i) \qquad y'_{i+1} = f(t_{i+1}, y^0_{i+1})$$

$$y_{i+1} \approx y_i + \frac{1}{2}(K_1 + K_2)$$

$$K_1 = hf(t_i, y_i)$$

$$K_2 = hf(t_i + h, y_i + K_1)$$

Average slopes: $\bar{y}' = \frac{y'_i + y'_{i+1}}{2} = \frac{f(t_i, y_i) + f(t_{i+1}, y^0_{i+1})}{2}$

Explicit form: $\boxed{y_{i+1} = y_i + \bar{y}'h = y_i + \frac{f(t_i, y_i) + f(t_{i+1}, y^0_{i+1})}{2}h = y_i + \frac{h}{2}(f(t_i, y_i) + f(t_{i+1}, y_i + hf(t_i, y_i)))}$

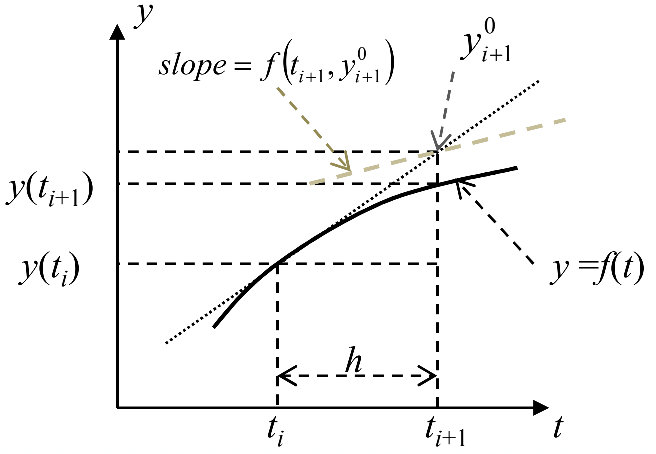
Predictor-corrector approach form:

Predictor: $y^0_{i+1} = y_i + hf(t_i, y_i)$

Corrector: $y_{i+1} = y_i + \frac{f(t_i, y_i) + f(t_{i+1}, y^0_{i+1})}{2}h$

$\underbrace{\qquad\qquad}$

Predictor is basic Euler method



Ordinary differential equations (ODEs)

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

Improved Euler method – Heun’s method (Predictor-corrector method)

$y(x=1)=?$

E.g. $\boldsymbol{y'=4e^{0.8x}-0.5y}$, $0\le x\le 4$, 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 (Predictor-corrector method)

$$y_{i+1} \approx y_i + \frac{1}{2}(K_1 + K_2)$$

$$K_1 = hf(t_i, y_i)$$

$$K_2 = hf(t_i + h, y_i + K_1)$$

		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!

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

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

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

Local error

Trapezoidal rule for integration

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

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)

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

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

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

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

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

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

$$\boxed{\begin{aligned} &X''(t) = {}^{d}\!/_{dt}\, F\left(t, X\right) \\ &x_1(t),\ x_2(t), \cdots \end{aligned}}$$

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

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

$$X(t+h) \approx X(t) + hX'(t) + \frac{h^2}{2!}X''(t) + O(h^3) \dashleftarrow$$

Second-order Taylor series method

$$X(t+h) \approx X(t) + hX'(t) + O(h^2) \dashleftarrow$$

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

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

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

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

Maximum-magnitude -----→ $\|E\|_\infty = \max\limits_{1\le i\le n} |e_i| = \max\left(|0.883131|, |0.430858|\right) = 0.883131$

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. : $\mathbf{x'=x+4y-e^t}$, $\mathbf{y'=x+y+2e^t}$.
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 $\mathbf{x=4e^{3t}+2e^{-t}-2e^t}$, $\mathbf{y=2e^{3t}-e^{-t}+1/4\ e^t}$. $x(0.2)=6.483131$, $y(0.2)=3.130858$.
Here, $h=0.2$, $t=0$.

Try RK2 Heun

$$X_{i+1} \approx X_i + \frac{1}{2}(K_1+K_2)$$

$$K_1 = hF(t_i, X_i)$$

$$K_2 = hF(t_i+h, X_i+K_1)$$

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

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

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

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

$$X(0.2) = X(0) + 1/6(F_1+2F_2+2F_3+F_4) = \begin{bmatrix} 4 \\ 5/4 \end{bmatrix} + 1/6\left(\begin{bmatrix} 1.6 \\ 1.45 \end{bmatrix} + 2\begin{bmatrix} 2.318966 \\ 1.797068 \end{bmatrix} + 2\begin{bmatrix} 2.52969 \\ 1.903672 \end{bmatrix} + \begin{bmatrix} 3.584595 \\ 2.425234 \end{bmatrix}\right) = \begin{bmatrix} 6.480318 \\ 3.129452 \end{bmatrix}.$$

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)

Systems of first-order initial value problems

Exercise: $\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + y = 2x^2 - 1$

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

Exact solution: $ae^x + bxe^x + 2x^2 + 8x + 11.$

Initial value problem: $y(0)=1, y'(0)=2,$
$y = -10e^x + 4xe^x + 2x^2 + 8x + 11.$

Try using RK2 Heun

$$X_{i+1} \approx X_i + \frac{1}{2}(K_1 + K_2)$$
$$K_1 = hF(t_i, X_i)$$
$$K_2 = hF(t_i + h, X_i + K_1)$$

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