Numerical Integration of ODEs

Kostas Kokkotas

December 9, 2019

Eberhard Karls Univerity of Tübingen

Single Step Methods

Single Step Methods : Taylor series

The numerical solution of the ODE

$$y' = f(x, y) \quad \text{with} \quad y(x_0) = y_0 \tag{1}$$

at a given point x can be found by finding the coefficients of the Taylor series expansion about the initial point x_0. More specifically:

$$y(x) = y(x_0 + h) = y(x_0) + hy'(x_0) + \frac{h^2}{2} y''(x_0) + \cdots \tag{2}$$

where $h = x - x_0$.

Thus we need to provide the "coefficients":

$$y'' = f'(x, y), \quad y''' = f''(x, y), \ldots \tag{3}$$

Taylor series : Example i

We will find the $y(1)$ for the ODE

$$y' = x + y \quad \text{with} \quad y(x_0) = 1 \quad \text{where} \quad x_0 = 0\,. \tag{4}$$

$$\begin{aligned}
y'(x_0) &= y'(0) = 0 + 1 = 1 \\
y'' &= 1 + y' = 1 + x + y = 1 + y' \\
y''(x_0) &= 1 + y'(0) = 2 \\
y''' &= 1 + y' \\
y'''(x_0) &= 1 + y'(0) = 2 \\
y^{(4)} &= 1 + y' \\
y^{(4)}(x_0) &= 1 + y'(0) = 2
\end{aligned}$$

Thus

$$y(0+h) = 1 + h + h^2 + \frac{h^3}{3} + \frac{h^4}{12} + \cdots \tag{5}$$

Taylor series : Example ii

and the error will be

$$E = \frac{y^{(5)}(\xi)}{5!} h^5 \quad \text{for} \quad 0 < \xi < h \tag{6}$$

x	y	Analytic	Error	Error $(h = 0.1)$
0	1	1		
0.1	1.110342	1.110342	1.7×10^{-7}	1.7×10^{-7}
0.2	1.24280	1.24281	5.5×10^{-6}	3.7×10^{-7}
0.3	1.39968	1.39972	4.3×10^{-5}	6.2×10^{-7}
0.4	1.383467	1.383649	1.8×10^{-4}	9.1×10^{-7}
:				
1.0	3.416667	3.436564	2×10^{-2}	4.2×10^{-6}

Table 1: Error in 3rd column assuming a $h = x$, Error in 4th column assuming step $h = 0.1$

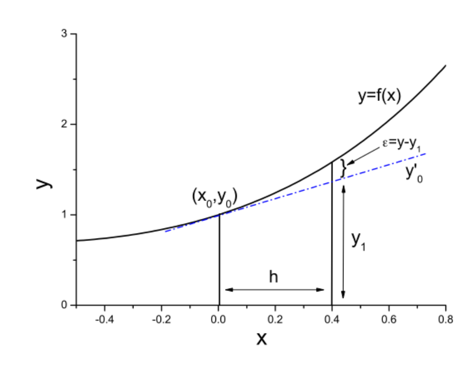
Single Step Methods : Euler-Heun

- **EULER** We keep only the 1st term of the Taylor series:

$$y(x_0 + h) = y(x_0) + hy'(x_0) \qquad (7)$$

with and obvious error:

$$E = \frac{y''(\xi)}{2} h^2 \quad \text{for} \quad 0 < \xi < h$$



- **EULER - HEUN** : This is a **predictor - corrector** method

$$\text{1st step :} \quad y_{n+1} = y_n + hy'_n + O(h^2) \qquad (8)$$

$$\text{2nd step :} \quad y_{n+1} = y_n + \frac{h}{2}\left(y'_n + y'_{n+1}\right) + O(h^3) \qquad (9)$$

Can you explain the smaller error?

Propagation of Errors

- If we consider the first order ODE $y' = f(x, y)$, with $y(x_0) = y_0$ then if Y_n is the calculated value at x_n and y_n the true value at x_n the error at x_n will be

$$\varepsilon_n = y_n - Y_n \tag{10}$$

- Let's try to study the propagation of the error for the Euler method:

$$\begin{aligned}
\varepsilon_{n+1} &= y_{n+1} - Y_{n+1} = \left[y_n + h \cdot f\left(x_n, y_n\right)\right] - \left[Y_n + h \cdot f\left(x_n, Y_n\right)\right] \\
&= \varepsilon_n + h \frac{\left[f\left(x_n, y_n\right) - f\left(x_n, Y_n\right)\right]}{y_n - Y_n} \varepsilon_n = \varepsilon_n \left[1 + h \cdot f_y\left(x_n, y_n\right)\right] \\
&= \left(1 + h \cdot k_n\right) \varepsilon_n + \frac{1}{2} h^2 y''\left(\xi_n\right) \quad \text{where} \quad k_n = \left(\frac{\partial f}{\partial y}\right)_{x = x_n},
\end{aligned} \tag{11}$$

implying that the propagation of the error is linear.

- If $|1 + hk_n| \geq 1$ the error **increases** while if $|1 + hk_n| \leq 1$ the error **decreases**.
- This leads to the necessary condition for **absolute convergence**:

$$-2 < hk_n < 0 \quad \text{or} \quad \left(\frac{\partial f}{\partial y}\right)_{x = x_n} < 0. \tag{12}$$

Convergence

Lets assume an ODE of the form

$$\frac{dy}{dx} = Ay \tag{13}$$

which has an obvious solution of the form $y = e^{Ax}$.
Euler's method gives the approximate solution via the recurrence relation:

$$y_{n+1} = y_n + hAy_n = (1 + hA)y_n \quad \text{for} \quad n = 0, 1, 2, \dots \tag{14}$$

Thus if we use this relation n-times we will get:

$$y_{n+1} = (1 + hA)^{n+1} y_0 \quad \text{for} \quad n = 0, 1, 2, \dots \tag{15}$$

But for small h we know that $1 + hA \approx e^{hA}$ thus

$$y_{n+1} = (1 + hA)^{n+1} y_0 \approx e^{(n+1)hA} y_0 = e^{(x_{n+1} - x_0)A} y_0 = e^{Ax_{n+1}} \tag{16}$$

where $h = (x_{n+1} - x_0)/(n + 1)$.

This means that the numerical solution for small h converges to the analytic solution: $y = e^{Ax}$.

Runge - Kutta Methods i

Let's assume the ODE

$$\frac{dy}{dx} = f\left(x, y\right) \tag{17}$$

A possible recurrence relation for the estimation of y_n can be of the form

$$y_{n+1} = y_n + ak_1 + bk_2 \tag{18}$$

where

$$\begin{aligned} k_1 &= hf\left(x_n, y_n\right) & (19) \\ k_2 &= hf\left(x_n + Ah, y_n + Bk_1\right) & (20) \end{aligned}$$

Let's try to find the equivalent Taylor expansion we get

$$y_{n+1} = y_n + hf\left(x_n, y_n\right) + \frac{h^2}{2} f'\left(x_n, y_n\right) + O(h^3) \tag{21}$$

But since

$$\frac{df}{dx} = f_x + f_y \frac{dy}{dx} = f_x + f_y f \tag{22}$$

Runge - Kutta Methods ii

we get

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2}\left(f_x + ff_y\right)_{x=x_n} \tag{23}$$

By comparing with (18), which can be written as:

$$y_{n+1} = y_n + ahf\left(x_n, y_n\right) + bhf\left[x_n + Ah, y_n + Bhf\left(x_n, y_n\right)\right] \tag{24}$$

we can get the Taylor series [1] expansion

$$y_{n+1} = y_n + h\left(a + b\right) f_n + h^2\left(A\, b\, f_x + B\, b\, f\; f_y\right)_n \tag{25}$$

thus we get the following relations for the arbitrary constants a, b, A and B :

$$a + b = 1, \qquad A \cdot b = \frac{1}{2} \quad \text{and} \quad B \cdot b = \frac{1}{2} \tag{26}$$

By setting $a = \frac{2}{3}, \frac{1}{2}, \frac{5}{4}\ \ldots$ we can estimate the other 3 unknowns.

Here, for simplicity we choose $a = \frac{1}{2}$ then $b = \frac{1}{2}$ and $A = B = 1$, i.e.

$$y_{n+1} = y_n + \frac{1}{2}(k_1 + k_2) \tag{27}$$

where

$$k_1 = hf\left(x_n, y_n\right), \quad k_2 = hf\left(x_n + h, y_n + k_1\right) \tag{28}$$

which is Euler-Heun's method !!!

[1] Here we use: $f\left(x_n + Ah, y_n + Bhf\left(x_n, y_n\right)\right) \approx \left(f + f_x Ah + f_y Bhf\right)_{x=x_n}$

3rd order Runge - Kutta Method

In a similar way we can derive the **3rd order Runge-Kutta** method:

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3\right) + O(h^4) \tag{29}$$

where

$$\begin{aligned} k_1 &= hf\left(x_n, y_n\right) & (30)\\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) & (31)\\ k_3 &= hf\left(x_n + h, y_n + 2k_2 - k_1\right) & (32)\\ && (33) \end{aligned}$$

This method if $f = f(x)$ i.e. independent of y reduces to Simpson's method.

Exercise: See in the exercises a different writing of the 3rd order RK method and try to prove it.

4th order Runge - Kutta Method

- If we repeat the same procedure for a Taylor series up to h^4, we will create a system of 11 equations with 13 unknowns.
- Then with the appropriate choice of two of them we come to a recurrence relation of the form :

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{34}$$

where

$$\begin{aligned} k_1 &= hf\left(x_n, y_n\right) && (35)\\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) && (36)\\ k_3 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right) && (37)\\ k_4 &= hf\left(x_n + h, y_n + k_3\right) && (38) \end{aligned}$$

This the 4th order **Runge - Kutta** with local error $E \approx O(h^5)$ and global error after n steps $E \approx O(h^4)$.

4th order Runge - Kutta - Merson Method

In this method the order is not given by the number of k's, but by the global error:

$$\begin{aligned}
k_1 &= hf\left(x_n, y_n\right) && (39)\\
k_2 &= hf\left(x_n + \frac{1}{3}h, y_n + \frac{1}{3}k_1\right) && (40)\\
k_3 &= hf\left(x_n + \frac{1}{3}h, y_n + \frac{1}{6}k_1 + \frac{1}{6}k_2\right) && (41)\\
k_4 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{8}k_1 + \frac{3}{8}k_3\right) && (42)\\
k_5 &= hf\left(x_n + h, y_n + \frac{1}{2}k_1 - \frac{3}{2}k_3 + 2k_4\right) && (43)
\end{aligned}$$

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 4k_4 + k_5\right) + O\left(h^5\right) \tag{44}$$

ERROR:

$$\mathcal{E} = \frac{1}{30}\left(2k_1 - 9k_3 + 8k_4 - k_5\right) \tag{45}$$

Runge - Kutta - Fehlberg Method i

$$
\begin{aligned}
k_1 &= hf\left(x_n, y_n\right) && (46)\\
k_2 &= hf\left(x_n + \frac{1}{4}h, y_n + \frac{1}{4}k_1\right) && (47)\\
k_3 &= hf\left(x_n + \frac{3}{8}h, y_n + \frac{3}{32}k_1 + \frac{9}{32}k_2\right) && (48)\\
k_4 &= hf\left(x_n + \frac{12}{13}h, y_n + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3\right) && (49)\\
k_5 &= hf\left(x_n + h, y_n + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4\right) && (50)\\
k_6 &= hf\left(x_n + \frac{1}{2}h, y_n - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5\right) && (51)
\end{aligned}
$$

Then a first estimation for y_{n+1} is:

$$\overline{y}_{n+1} = y_n + \left(\frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5\right) \tag{52}$$

Runge - Kutta - Fehlberg Method ii

here the local error is $\approx h^5$.

The next step will include k_6 and gives:

$$y_{n+1} = y_n + \left(\frac{16}{135} k_1 + \frac{6656}{12825} k_3 + \frac{28561}{56430} k_4 - \frac{9}{50} k_5 + \frac{2}{55} k_6 \right) \tag{53}$$

with local error $\approx h^6$ and global $\approx h^5$.

A formula for the estimation of error of the Runge - Kutta - Fehlberg method is

$$\mathcal{E} = \frac{1}{360} k_1 - \frac{128}{4275} k_3 - \frac{2197}{7524} k_4 + \frac{1}{50} k_5 + \frac{2}{55} k_6 \tag{54}$$

Since the $k_1, k_2, \ldots, k_6$ are known in every step we can always test the accuracy of the method and if is worst than the demanded we subdivide the step h.

- See an extensive analysis in:

http://www.mathematik.uni-stuttgart.de/studium/infomat/Numerische-Mathematik-II-SS11/Matlab/ode_4.pdf

Multistep Methods

Adams's Method i

- The principle behind a multistep method is to utilize the past values of y and/or y' to construct a polynomial that approximates the derivative function, and extrapolate this into the next interval.
- The number of past points that are used sets the degree of the polynomial and is therefore responsible for the truncation error.
- The order of the method is equal to the power of h in the global error term of the formula, which is also equal to one more than the degree of the polynomial.
- We will write the ODE in the form:

$$\frac{dy}{dx} = f(x, y) \quad \text{then} \quad dy = f(x, y)\, dx \tag{55}$$

and then we integrate between x_n and x_{n+1} :

$$\int_{x_n}^{x_{n+1}} dy = y_{n+1} - y_n = \int_{x_n}^{x_{n+1}} f(x, y)\, dx \tag{56}$$

Adams's Method ii

We can use the trapezoidal rule for the integration

$$y_{n+1} - y_n = \int_{x_n}^{x_{n+1}} f(x, y)\, dx = \frac{h}{2}\left[f(x_n, y(x_n)) + f(x_n + h, y(x_n + h))\right] + \frac{h^3}{12} f''(\xi) \tag{57}$$

thus the new scheme will be:

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_n + y'_{n+1}\right) - \frac{h^3}{12} y'''(\xi) \tag{58}$$

alternatively:

$$\begin{aligned} y_{n+1} &= y_n + h y'_n + \frac{1}{2} y''_n h^2 + \frac{h^3}{6} y'''(\xi) \\ &= y_n + h y'_n + \frac{1}{2}\left[\frac{y'_{n+1} - y'_n}{h} - \frac{h}{2} y'''(\xi)\right] h^2 + \frac{h^3}{6} y'''(\xi) \\ &= y_n + \frac{1}{2}\left(y'_n + y'_{n+1}\right) - \frac{h^3}{12} y'''(\xi) \end{aligned} \tag{59}$$

Did you ever met this relation again?

Adams's Method iii

NOTE: Can you prove the following expression?

$$y_{n+1} = y_n + \frac{h}{12}\left(5y'_{n+1} + 8y'_n - y'_{n-1}\right) - \frac{h^4}{24}y^{(4)} \tag{60}$$

or

$$y_{n+1} = y_n + \frac{h}{12}\left(5f_{n+1} + 8f_n - f_{n-1}\right) - \frac{h^4}{24}y^{(4)} \tag{61}$$

HINT

The previous relations suggest that we can use (appropriately) the methods that we developed for the numerical evaluation of integrals in order to derive more accurate relations.

The typical way was to integrate the term on the right of (56) by using an approximate form of $f(x, y)$ e.g. using an interpolating polynomial in x.

NOTE: In deriving this we have to use several "past points".

3rd order Adams's Method i

Here we use quadratic approximation

$$\begin{aligned}
\int_{x_n}^{x_{n+1}} dy &= y_{n+1} - y_n \\
&= \int_{x_n}^{x_{n+1}} \left[f_n + s\Delta f_{n-1} + \frac{(s+1)\,s}{2}\Delta^2 f_{n-2} + \text{Error} \right] dx \\
&= h \int_{s=0}^{s=1} \left[f_n + s\Delta f_{n-1} + \frac{(s+1)s}{2}\Delta^2 f_{n-2} \right] ds \\
&\quad + h \int_{s=0}^{s=1} \frac{s(s+1)(s+2)}{6} h^3 f'''(\xi) ds
\end{aligned}$$

then

$$\begin{aligned}
y_{n+1} - y_n &= h\left[f_n + \frac{1}{2}\Delta f_{n-1} + \frac{5}{12}\Delta^2 f_{n-2} \right] + O\left(h^4\right) \\
&= h\left[f_n + \frac{1}{2}\left(f_n - f_{n-1}\right) + \frac{5}{12}\left(f_n - 2f_{n-1} + f_{n-2}\right) \right] + O\left(h^4\right)
\end{aligned}$$

$$y_{n+1} = y_n + \frac{h}{12}\left[23f_n - 16f_{n-1} + 5f_{n-2}\right] + \frac{3}{8}h^4 f'''(\xi) \qquad (62)$$

3rd order Adams's Method ii

If we use cubic approximation we get:

$$y_{n+1} = y_n + \frac{h}{24}\left[55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}\right] + O\left(h^5\right) \tag{63}$$

ERROR TERM : We get the error term of the 4th order Adams formula by integrating the error of the cubic interpolating polynomial

$$\mathcal{E} \approx \frac{251}{720} h^5 y^{(5)}(\xi), \qquad x_{n-3} \leq \xi \leq x_{n+1} \tag{64}$$

Milne's Method

This is an alternative method to Adams. We follow the same procedure but we use different limits of integration. Thus the ODE

$$\frac{dx}{dy} = f(x, y) \tag{65}$$

can be written as:

$$\int_{x_{n-3}}^{x_{n+1}} dy = y_{n+1} - y_{n-3} = \int_{x_{n-3}}^{x_{n+1}} f(x, y)\, dx \tag{66}$$

and if we replace $f(x, y)$ with a 2nd order polynomial

$$y_{n+1} = y_{n-3} + \frac{4h}{3}\left(2f_n - f_{n-1} + 2f_{n-2}\right) + O\left(h^5\right) \tag{67}$$

ERROR TERM

$$\mathcal{E} \approx \frac{28}{90} h^5 y^{(5)}(\xi), \qquad x_{n-3} \leq \xi \leq x_{n+1} \tag{68}$$

Predictor - Corrector Methods

Predictor - Corrector Methods i

We estimate the value of $y_{k+1} = y(x_{k+1})$ by using two successive approximations.

Prediction : we use the m previous points

$$y_{k+1} = \mathcal{P}\left(y_{k-m}, y_{k-m+1}, \dots, y_k\right) \tag{69}$$

Correction : we include the "predicted" value of y_{k+1}

$$y_{k+1} = \mathcal{C}\left(y_{k-m}, y_{k-m+1}, \dots, y_k, y_{k+1}\right) \tag{70}$$

This 2nd step **can be repeated a few times** until the two "corrected" values converge i.e. until

$$\left| y_{k+1}^{(j)} - y_{k+1}^{(j+1)} \right| < \mathcal{E}$$

where j is the number of iterations and $\mathcal{E}$ is the maximum allowed error.

Predictor - Corrector Methods : Milne - Simpson

A corrector formula for Milne's method can be derived by just shifting the integration limits

$$\int_{x_{n-1}}^{x_{n+1}} dy = y_{n+1} - y_{n-1} = \int_{x_{n-1}}^{x_{n+1}} f\left(x, y\right) dx \tag{71}$$

and by using Simpson's rule for the integral we get

$$y_{n+1} = y_{n-1} + \frac{h}{3}\left(f_{n+1} + 4f_n + f_{n-1}\right) \tag{72}$$

with error:

$$\mathcal{E} \approx \frac{h^5}{90} y^{(5)}\left(\xi\right) \quad \text{where} \quad x_{n-1} < \xi < x_{n+1} \tag{73}$$

Milne's Predictor-Corrector formulas

$$y_{k+1} = y_{k-3} + \frac{4h}{3}\left(2f_{k-2} - f_{k-1} + 2f_k\right) + \frac{28}{90} h^5 y^{(5)}(\xi_1) \quad \left(x_{k-3} < \xi_1 < x_{k+1}\right) \tag{74}$$

$$y_{k+1} = y_{k-1} + \frac{h}{3}\left(f_{k-1} + 4f_k + f_{k+1}\right) - \frac{1}{90} h^5 y^{(5)}(\xi_2) \quad \left(x_{k-1} < \xi_2 < x_{k+1}\right) \tag{75}$$

PREDICTION $(x_{k-3} < \xi_1 < x_{k+1})$

$$y_{k+1} = y_k + \frac{h}{24}\left(55f_k - 59f_{k-1} + 37f_{k-2} - 9f_{k-3}\right) + \frac{251}{720}h^5 y^{(5)}(\xi_1) \tag{76}$$

CORRECTION $(x_{k-2} < \xi_2 < x_{k+1})$

$$y_{k+1} = y_k + \frac{h}{24}\left(9f_{k+1} + 19f_k - 5f_{k-1} + f_{k-2}\right) - \frac{19}{720}h^5 y^{(5)}(\xi_2) \tag{77}$$

NOTE The correction formula can be derived assuming integration from x_k to x_{k+1} and demanding as in Gauss integration method that the formula is exact for 3rd order polynomials and using the points x_{k+1}, x_k, x_{k-1} and x_{k-2}. In this way we will get the formula:

$$\int_{x_k}^{x_{k+1}} f(t)dt \approx \frac{h}{24}\left(9f_{k+1} + 19f_k - 5f_{k-1} + f_{k-2}\right) \tag{78}$$

In a similar way one may derive also the correction term using Gauss method for the points x_k, x_{k-1}, x_{k-2} and x_{k-3}. Even thought using Newtons interpolating polynomial it is easier, as it was shown earlier.

Predictor - Corrector Methods : Hamming

The Hamming method (1959) is a stable predictor-corrector method for ODEs. It was developed for replacing the classical Milne - Simpson method by replacing unstable corrector rule by a stable one.

PREDICTION $(x_{k-3} < \xi_1 < x_{k+1})$[2]

$$y_{k+1} = y_{k-3} + \frac{4h}{3}\left(2f_{k-2} - f_{k-1} + 2f_k\right) + \frac{14}{45}h^5 y^{(5)}(\xi_1) \tag{79}$$

CORRECTION $(x_{k-2} < \xi_2 < x_{k+1})$

$$y_{k+1} = \frac{1}{8}\left(9y_k - y_{k-2}\right) + \frac{3h}{8}\left(-f_{k-1} + 2f_k + f_{k+1}\right) - \frac{1}{40}h^5 y^{(5)}(\xi_1) \tag{80}$$

[2] It is Milne's prediction formula

Systems of ODE

For the numerical solution of systems of ODEs we follow the methods developed earlier.

For example, the 4th order Runge-Kutta will look like:

$$y_{n+1} = y_n + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{81}$$

$$z_{n+1} = z_n + \frac{1}{6}\left(l_1 + 2l_2 + 2l_3 + l_4\right) \tag{82}$$

where

$$k_1 = h\,f(x_n, y_n, z_n) \tag{83}$$

$$k_2 = h\,f\left(x_n + \frac{1}{2}h,\, y_n + \frac{1}{2}k_1,\, z_n + \frac{1}{2}l_1\right) \tag{84}$$

$$k_3 = h\,f\left(x_n + \frac{h}{2},\, y_n + \frac{1}{2}k_2,\, z_n + \frac{1}{2}l_2\right) \tag{85}$$

$$k_4 = h\,f\left(x_n + h,\, y_n + k_3,\, z_n + l_3\right) \tag{86}$$

$$l_1 = h\,g(x_n, y_n, z_n) \tag{87}$$

$$l_2 = h\,g(x_n + \frac{1}{2}h,\, y_n + \frac{1}{2}k_1,\, z_n + \frac{1}{2}l_1) \tag{88}$$

$$l_3 = h\,g\left(x_n + \frac{1}{2}h,\, y_n + \frac{1}{2}k_2,\, z_n + \frac{1}{2}l_2\right) \tag{89}$$

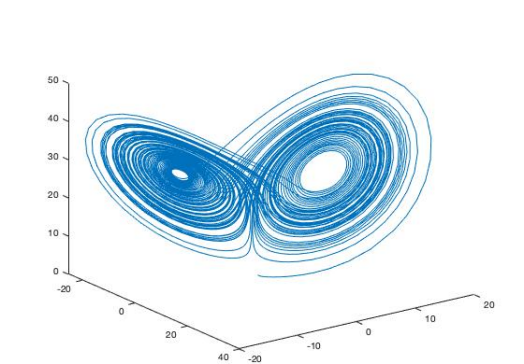
$$l_4 = h\,g\left(x_n + h,\, y_n + k_3,\, z_n + l_3\right) \tag{90}$$

Lorenz Attractor

The Lorenz attractor can be derived via the following systems ODEs

$$\begin{aligned} x' &= 10(y-x) && (91) \\ y' &= x(28-z)-y && (92) \\ z' &= xy - \frac{8}{3}z && (93) \end{aligned}$$

Here with the following initial conditions $x(0) = 1$, $y(0) = 0$, $z(0) = 0$ and $t = 0 \ldots 100$



Stiff Systems of ODEs

Instabilities in the numerical schemes i

We show that Milne's method can become unstable even for simple ODEs.

Consider the ODE

$$\frac{dy}{dx} = Ay \quad \text{with general solution for} \quad x = x_n \quad \text{the} \quad y_n = y_0 e^{A(x_n - x_0)}$$

If we solve this ODE with Milne's method we will use the **corrector** formula

$$y_{n+1} = y_{n-1} + \frac{h}{3}\left(y'_{n+1} + 4y'_n + y'_{n-1}\right)$$

where by substituting $y'_n = Ay_n$ we get

$$y_{n+1} = y_{n-1} + \frac{h}{3}\left(Ay_{n+1} + 4Ay_n + Ay_{n-1}\right)$$

and by rearranging, we get

$$\left(1 - \frac{hA}{3}\right) y_{n+1} - \frac{4hA}{3} y_n - \left(1 + \frac{hA}{3}\right) y_{n-1} = 0$$

This is a 2nd order *difference equation*.

Instabilities in the numerical schemes ii

The difference equation admits a solution of the form

$$y_n = c_1 Z_1^n + c_2 Z_2^n$$

where Z_1 and Z_2 are the roots of the quadratic equation:

$$\left(1 - \frac{hA}{3}\right) Z^2 - \frac{4hA}{3} Z - \left(1 + \frac{hA}{3}\right) = 0$$

If we set $r = hA/3$

$$(1 - r)\, Z^2 - 4rZ - (1 + r) = 0$$

the roots of the above quadratic equation will be

$$\begin{aligned} Z_1 &= \frac{2r + \sqrt{3r^2 + 1}}{1 - r} \approx 1 + 3r \approx e^{3r} + O(r^2) = e^{hA} \\ Z_2 &= \frac{2r - \sqrt{3r^2 + 1}}{1 - r} \approx -1 + r \approx -e^{-r} + O(r^2) = -e^{-hA/3} \end{aligned}$$

Instabilities in the numerical schemes iii

Hence the Milne solution is represented by

$$y_n = c_1 e^{nhA} + c_2 e^{-nhA/3} = c_1 e^{A(x_n - x_0)} + c_2 e^{-A(x_n - x_0)/3} \quad , x_n - x_0 = nh$$

- The 1st term is as expected
- The 2nd term is **parasitic** :
  - for $A > 0$ dies out as x_n increases, BUT
  - for $A < 0$ it will grow exponentially with x_n.

EXAMPLES

1. Solve numerically the ODE
   $y' = -10y$, with $y(0) = 1$
   from $x = 0$ to $x = 2$ by using Milne's and Adams-Multon's methods. What are your conclusions about the error?
2. Use Milne's method to solve numerically the ODE
   $y' = 2(x + 1)$, with $y(1) = 3$
   Is there any indication of instability?

Convergence Criteria i

We will look for a criterion to show how small h should be in the Adams-Multon method so that re-corrections are not necessary.
Let :

- y_p = value of y_{n+1} from predictor formula
- y_c = value of y_{n+1} from corrector formula
- $y_{cc}, y_{ccc}, \ldots$ = value of y_{n+1} if successive re-corrections are made,
- y_∞ = values to which successive re-corrections converge
- $D = y_c - y_p$

The change of y_c by re-correcting would be

$$\begin{aligned} y_{cc} - y_c \quad &= \quad \left[y_n + \frac{h}{24}\left(9y'_c + 19y'_n - 5y'_{n-1} + y'_{n-2}\right)\right] \\ &- \quad \left[y_n + \frac{h}{24}\left(9y'_p + 19y'_n - 5y'_{n-1} + y'_{n-2}\right)\right] = \frac{9h}{24}\left(y'_c - y'_p\right) \end{aligned}$$

Convergence Criteria ii

By manipulating the difference $(y'_c - y'_p)$ we get:

$$
\begin{aligned}
y'_c - y'_p &= f(x_{n+1}, y_c) - f(x_{n+1}, y_p) = \frac{f(x_{n+1}, y_c) - f(x_{n+1}, y_p)}{y_c - y_p}(y_c - y_p) \\
&= f_y(\xi_1)D \quad \text{where} \quad y_c \le \xi_1 \le y_p. \qquad (94)
\end{aligned}
$$

Hence

$$
y_{cc} - y_c = \frac{9h}{24}\left(y'_c - y'_p\right) = \frac{9h}{24} f_y(\xi_1)D \qquad (95)
$$

If recorrected again, the result is

$$
\begin{aligned}
y_{ccc} - y_{cc} &= \frac{9h}{24}(y'_{cc} - y'_c) = \frac{9h}{24} f_y(\xi_2)(y_{cc} - y_c) = \frac{9h}{24} f_y(\xi_2)\left[\frac{9hD}{24} f_y(\xi_1)\right] \\
&= \left(\frac{9h}{24}\right)^2 [f_y(\xi)]^2 D \qquad (96)
\end{aligned}
$$

Convergence Criteria iii

On further re-corrections we will have a similar relation. Finally, we get y_∞ by adding all the corrections of y_p together:

$$\begin{aligned} y_\infty &= y_p + (y_c - y_p) + (y_{cc} - y_c) + (y_{ccc} - y_{cc}) + \ldots \\ &= y_p + D + \frac{9hf_y(\xi)}{24} D + \left(\frac{9hf_y(\xi)}{24}\right)^2 D + \left(\frac{9hf_y(\xi)}{24}\right)^3 D + \ldots \\ &= y_p + D\left[1 + r + r^2 + r^3 + \ldots\right] = y_p + \frac{D}{1-r}, \end{aligned}$$

where

$$r = \frac{9h}{24} f_y(\xi).$$

The above geometrical series will converge only if the r is smaller than unity:

$$|r| = \frac{h|f_y(\xi)|}{24/9} = \frac{h|f_y(x_n, y_n)|}{24/9} < 1$$

Convergence Criteria - Adams-Multon Method

Thus the **1st convergence criterion** will be:

$$h < \frac{24/9}{|f_y(x_n, y_n)|}$$

If we wish to have y_c and y_∞ the same to within one in the Nth decimal places, then

$$y_\infty - y_c = \left(y_p + \frac{D}{1-r}\right) - (y_p + D) = \frac{rD}{1-r} < 10^{-N}$$

If $r \ll 1$ the fraction will be approximately $r/(1-r) \approx r$ we can write a **2nd convergence criterion** which ensures that the 1st corrected value is adequate (i.e. it will not changed in the Nth decimal place by further corrections)

$$D \cdot 10^N < \left|\frac{1}{r}\right| = \frac{24/9}{h|f_y(x_n, y_n)|}$$

Convergence Criteria - Milne Method

Similar criteria can be found for the Milne method :

1st convergence criterion :

$$h < \frac{3}{|f_y(x_n, y_n)|}$$

2nd convergence criterion :

$$D \cdot 10^N < \left|\frac{1}{r}\right| = \frac{3}{h|f_y(x_n, y_n)|}$$

NOTE: These criteria are for a single 1st order ODE only. A similar analysis for a system is much more complicated.

Typical Sources of Error

- The previous error analysis examined the error of a single step only, the so called **local truncation error**.
- The accumulation of these errors, termed as the **global truncation error** is important.

There are other sources of error in addition to the truncation error.

- **Original data errors :** If the initial conditions are not known exactly or exressed inexactly as terminated decimal number, the solution will be affected to a greater or lesser degree depending on the sensitivity of the equation.
- **Round-off errors :** Both floating-point and fixed-point calculations in computers are subject to round off errors.
- **Truncation errors of the method:** These are the types of error due to the use of truncated series for approximation in our work, when infinite series is needed for exactness.

Error Propagation i

When we solve ODEs numerically we must worry about the propagation of the previous errors through the subsequent steps.

If we consider the 1st order ODE $y' = f(x, y)$, with $y(x_0) = y_0$ then if Y_n is the calculated value at x_n and y_n the true value, then the error in Y_n will be:

$$\varepsilon_n = y_n - Y_n \tag{97}$$

By the Euler algorithm :

$$\begin{aligned}
\varepsilon_{n+1} &= y_{n+1} - Y_{n+1} = y_n + hf(x_n, y_n) - Y_n - hf(x_n, Y_n) + \frac{1}{2}h^2 y''(\xi_n) \\
&= \varepsilon_n + h\frac{f(x_n, y_n) - f(x_n, Y_n)}{y_n - Y_n}\varepsilon_n + \frac{1}{2}h^2 y''(\xi_n) \\
&= \varepsilon_n (1 + hf_y(x_n, \eta_n)) + \frac{1}{2}h^2 y''(\xi_n) \quad \text{where } \eta_n \text{ between } y_n,\ Y_n \\
&= (1 + hk)\varepsilon_n + \frac{1}{2}h^2 y''(\xi_n) \quad \text{where} \quad k = \frac{\partial f}{\partial y}.
\end{aligned} \tag{98}$$

Error Propagation ii

I.e. the error propagation is linear. If $|1 + hk| \geq 1$ the error increases while for $|1 + hk| \leq 1$ decreases. This observation leads to the condition:

$$-2 < hk < 0 \quad \text{or} \quad \partial f/\partial y < 0 \tag{99}$$

$$\varepsilon_{n+1} = (1 + hk)\,\varepsilon_n + \frac{1}{2}h^2 y''(\xi_n) \tag{100}$$

Since $Y_0 = y_0$ we get:

$$\begin{aligned}
\varepsilon_0 &= 0 \\
\varepsilon_1 &\leq (1 + hk)\varepsilon_0 + \frac{1}{2}h^2 y''(\xi_0) = \frac{1}{2}h^2 y''(\xi_0) \\
\varepsilon_2 &\leq (1 + hk)\left[\frac{1}{2}h^2 y''(\xi_0)\right] + \frac{1}{2}h^2 y''(\xi_1) = \frac{1}{2}h^2\left[(1 + hk)y''(\xi_0) + y''(\xi_1)\right] \\
\varepsilon_3 &\leq \frac{1}{2}h^2\left[(1 + hk)^2 y''(\xi_0) + (1 + hk)y''(\xi_1) + y''(\xi_2)\right] \\
\varepsilon_n &\leq \frac{1}{2}h^2\left[(1 + hk)^{n-1} y''(\xi_0) + (1 + hk)^{n-2} y''(\xi_1) + \ldots + y''(\xi_{n-1})\right]
\end{aligned}$$

Error Propagation iii

- If $k \geq 0$ the truncation error at every step is propagated to the next step after being "amplified" by the factor $(1 + hk)$. Finally, for $h \to 0$ the error at any point is the sum of all previous errors.
- If the f_y is negative and of magnitude such that $kh \leq 2$ the errors are propagated with diminishing effect. We now show that the **accumulated error** after n steps is $O(h)$; that is the global error of the simple Euler method after n steps is $O(h)$.

If $|y''(x)| < M$ with $M > 0$ then the previous equation will be written as:

$$|\varepsilon_{n+1}| \leq (1 + hk)|\varepsilon_n| + \frac{1}{2}h^2 M$$

which is a difference equations of the form:

$$Z_{n+1} = (1 + hk)Z_n + \frac{1}{2}h^2 M \quad \text{with} \quad Z_0 = 0$$

With obvious solution

Error Propagation iv

$$Z_n = \frac{hM}{2k}(1+hk)^n - \frac{hM}{2k}$$

since $1 + hk < e^{hk}$ for $k > 0$ we get

$$Z_n < \frac{hM}{2k}\left(e^{hk}\right)^n - \frac{hM}{2k} = \frac{hM}{2k}\left(e^{nhk} - 1\right) = \frac{hM}{2k}\left(e^{(x_n - x_0)k} - 1\right) = O(h)$$

It follows that the **global error** ε_n is $O(h)$

Comparison of the Numerical Methods

- **The advantages of Runge-Kutta method (single step)**
  - Easy application
  - Single-step i.e. no need for a "starting" method
  - Step-size can be changed during the integration to match accuracy needs (variable step-size)
- **Advantages of Multi-step & Predictor-Corrector Methods (Adams , . . .)**
  - More efficient than one-step methods (Adams-Moulton is about twice that of the Runge-Kutta-Felberg method) ☺
  - Local truncation error is easily estimated, so it can be adjusted.
  - Changes of step size with multistep methods is considerably more awkward. ☹