Numerical methods for ordinary differential equations

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Ordinary differential equations

The general first order equation can be written as:

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0, \tag{1}$$

with $f(x, y)$ given.
This is an Initial value problem (IVP).

Euler's Method

It is the simplest.
Choose step size h and $y(x_0) = y_0$ to generate $y(x_1), y(x_2), \ldots$ by sequence $y_i, i = 1, 2, \ldots$. Note $x_i = x_0 + ih$.
Taylor's expansion

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

Since $y'(x) = f(x, y)$ then $y'(x_i) = f(x_i, y_i)$, therefore

$$y(x+h) = y(x) + hf(x_i, y_i) + \frac{1}{2!}h^2 f_x(x_i, y_i) + \cdots$$

Truncate after the term in h and use notation $y(x_i) = y_i$ then

$$y_{i+1} = y_i + hf(x_i, y_i).$$

The truncation error is $\mathcal{O}(h^2)$:

$$E = \frac{h^2}{2!}y_i''(\xi), \quad \xi \in [x_i, x_{i+1}].$$

Example

Apply the Euler's method to solve the simple equation:

$$\frac{dy}{dx} = x + y, \qquad y(0) = 1$$

with $h = 0.1$ (Exercise: Solve the equation analytically and show that the analytic solution is $y = 2e^x - x - 1$.)

Solution:

Here $f(x_i, y_i) = x_i + y_i$. With $h = 0.1$, and $y_0 = 1$ so

$$\begin{aligned}
y_1 &= y_0 + hf(x_0, y_0) = 1 + 0.1(0 + 1) = 1.1 \\
y_2 &= y_1 + hf(x_1, y_1) = 1.1 + 0.1(0.1 + 1.1) = 1.220 \\
y_3 &= y_2 + hf(x_2, y_2) = 1.220 + 0.1(0.2 + 1.220) = 1.362 \\
y_4 &= y_3 + hf(x_3, y_3) = 1.362 + 0.1(0.3 + 1.362) = 1.528
\end{aligned}$$

So

$$y(0.1) = 1.1,\ y(0.2) = 1.220,\ y(0.3) = 1.362,\ y(0.4) = 1.528.$$

Midpoint Method

Euler method: $y_{i+1} = y_i + hf(x_i, y_i)$.
The Euler method assumes that $y'(x_i) = f(x_i, y_i)$ is the same for the whole interval $[x_i, x_{i+1}]$.
The midpoint uses Euler method to find y at the midpoint of $[x_i, x_{i+1}]$ ie.,

$$y_{i+\frac{1}{2}} = y_i + \frac{h}{2} f(x_i, y_i)$$

This is then used to find

$$y'(x_{i+\frac{1}{2}}) = f(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}})$$

This derivative is then used for the whole interval $[x_i, x_{i+1}]$.
So the Euler method becames

$$y_{i+1} = y_i + hy'(x_{i+\frac{1}{2}}) = y_i + hf(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}).$$

This is the midpoint rule and is $\mathcal{O}(h^3)$.
Note that $x_{i+\frac{1}{2}} = x_i + h/2$ but $y_{i+\frac{1}{2}} \neq y_i + h/2$.

Example

Apply the midpoint rule solve the equation:

$$\frac{dy}{dx} = x + y, \qquad y(0) = 1$$

with $h = 0.1$.

Solution:

Here $f(x_i, y_i) = x_i + y_i$. With $h = 0.1$, and $y_0 = 1$ also

$$y_{i+1} = y_i + hf(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}) = hf(x_i + \frac{h}{2}, y_i + \frac{h}{2} f(x_i, y_i)).$$

$$\begin{aligned}
y_1 &= y_0 + hf(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)) \\
&= 1 + 0.1f(0 + 0.05, 1 + 0.05f(0, 1)) = 1.110 \\
y_2 &= y_1 + hf(x_1 + \frac{h}{2}, y_1 + \frac{h}{2} f(x_1, y_1)) \\
&= 1.110 + 0.1f(0.1 + 0.05, 1.110 + 0.05f(0.1, 1.110)) \\
&= 1.24205
\end{aligned}$$

Error of Midpoint rule

The truncation error is $\mathcal{O}(h^3)$:

$$E = -\frac{h^3}{12} y_i'''(\xi), \quad \xi \in [x_i, x_{i+1}].$$

Runge-Kutta Methods

The general form of the Runge-Kutta method is:

$$y_{i+1} = y_i + \phi(x_i, y_i; h), \tag{2}$$

where $\phi(x_i, y_i; h)$ is called the increment function.
For Euler's method, $\phi(x_i, y_i; h) = hf(x_i, y_i) = hy_i'$
In the midpoint

$$\phi(x_i, y_i; h) = hf(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}) = hy'_{i+\frac{1}{2}}$$

The increment function can be written in a general form as:

$$\phi = w_1 k_1 + w_2 k_2 + \cdots + w_n k_n \tag{3}$$

where the k's are constants and the w's are weights and $w_1 + w_2 + \cdots + w_n = 1$

Second order Runge-Kutta Methods

The second order R-K method has the form:

$$y_{i+1} = y_i + (w_1 k_1 + w_2 k_2), \tag{4}$$

where

$$\begin{aligned} k_1 &= hf(x_i, y_i) && (5) \\ k_2 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}), && (6) \end{aligned}$$

and the weights $w_1 + w_2 = 1$.
If $w_1 = 1$, then $w_2 = 0$ and we have Euler's method.
If $w_1 = 0$, then $w_2 = 1$ we have the mipoint rule:

$$y_{i+1} = y_i + hf(x_i + \tfrac{h}{2}, y_i + \tfrac{k_1}{2}), \tag{7}$$

If $w_1 = w_2 = 1/2$, then we have:

$$y_{i+1} = y_i + \frac{1}{2}(k_1 + k_2) = y_i + \frac{h}{2}\left(f(x_i, y_i) + f\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)\right),$$

called Heun's method.

Fourth Order Runge-Kutta Methods

The **classical fourth order R-K method** has the form:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4), \tag{8}$$

where

$$\begin{aligned}
k_1 &= hf(x_i, y_i) && (9)\\
k_2 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}) && (10)\\
k_3 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}) && (11)\\
k_4 &= hf(x_i + h, y_i + k_3), && (12)
\end{aligned}$$

This is the most popular R-K method. It has a local truncation error $\mathcal{O}(h^4)$.

Example

Solve

$$y' = x + y, \quad y(0) = 1.$$

using 4^{th} order Runge-Kutta method. Compare your results with those obtained from Euler's method, midpoint method and the actual value. Determine $y(0.1)$ and $y(0.2)$ only.
The solution using Runge-Kutta is obtained as follows:
For y_1 :

$$\begin{aligned} k_1 &= hf(x_i, y_i) \\ &= 0.1(0+1) = 0.1 \\ k_2 &= hf(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}) \\ &= 0.1\left(\left(0 + \frac{0.1}{2}\right) + \left(1 + \frac{0.1}{2}\right)\right) = 0.11 \end{aligned}$$

Example cnt'd

$$
\begin{aligned}
k_3 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right) \\
&= 0.1\left(\left(0 + \frac{0.1}{2}\right) + \left(1 + \frac{0.11}{2}\right)\right) = 0.1105 \\
k_4 &= hf(x_i + h, y_i + k_3) \\
&= 0.1((0 + 0.1) + (1 + 0.1105)) = 0.1211
\end{aligned}
$$

and therefore:

$$y_1 = y_0 + \frac{1}{6}(0.1 + 2(0.11) + 2(0.1105) + 0.1211) = 1.1103$$

A similar computation yields

$$y_2 = 1.1103 + \frac{1}{6}(0.1210 + 2(0.1321) + 2(0.1326) + 0.1443 = 1.2428$$

Therefore $y(0.1) = 1.1103$ and $y(0.2) = 1.2428$

Comparison of all the methods so far

A table for all the approximate solutions using the required methods is:

x_i	Euler	Midpoint	4^{th} Order RK	Actual value
0.1	1.1000000	1.1100000	1.1103417	1.1103418
0.2	1.2300000	1.2420500	1.2428052	1.2428055

Systems of First Order ODEs

So far we have solved a single first order ODE for $y(x)$.
A nth order system of first order initial value problems can be expressed in the form:

$$\begin{aligned}
\frac{dy_1}{dx} &= f_1(x, y_1, y_2, \cdots, y_n), \quad y_1(x_0) = \alpha_1 \\
\frac{dy_2}{dx} &= f_2(x, y_1, y_2, \cdots, y_n), \quad y_2(x_0) = \alpha_2 \\
&\vdots \\
\frac{dy_n}{dx} &= f_n(x, y_1, y_2, \cdots, y_n), \quad y_n(x_0) = \alpha_n,
\end{aligned}$$

All the methods we have seen can used to solve first order systems of IVPs.
We seek n solutions $y_1,\ y_2, \ldots, y_n$ each with an intial condition $y_k(x_i); k = 1, \ldots, n$ at the points $x_i,\ i = 1, 2. \ldots .$

4^{th} order Runge-Kutta for systems of ODEs

Consider the system of two equations:

$$\frac{dy}{dx} = f(x, y, z), \quad y(0) = y_0 \tag{13}$$

$$\frac{dz}{dx} = g(x, y, z), \quad z(0) = z_0. \tag{14}$$

Let $y = y_1,\ z = y_2,\ f = f_1,$ and $g = f_2$. The fourth order R-K method would be applied as follows. For each $j = 1, 2$ corresponding to solutions $y_{j,i}$, compute

$$k_{1,j} = hf_j(x_i, y_{1,i}, y_{2,i}), \quad j = 1, 2 \tag{15}$$

$$k_{2,j} = hf_j(x_i + \frac{h}{2},\ y_{1,i} + \frac{k_{1,1}}{2},\ y_{2,i} + \frac{k_{1,2}}{2}) \quad j = 1, 2 \tag{16}$$

$$k_{3,j} = hf_j(x_i + \frac{h}{2},\ y_{1,i} + \frac{k_{2,1}}{2},\ y_{2,i} + \frac{k_{2,2}}{2}), \quad j = 1, 2 \tag{17}$$

$$k_{4,j} = hf_j(x_i + h,\ y_{1,i} + k_{3,1},\ y_{2,i} + k_{3,2}), \quad j = 1, 2 \tag{18}$$

4^{th} order Runge-Kutta for systems of ODEs

So for the system:

$$
\begin{aligned}
\frac{dy}{dx} &= f(x, y, z), \quad y(0) = y_0 && (19)\\
\frac{dz}{dx} &= g(x, y, z), \quad z(0) = z_0. && (20)
\end{aligned}
$$

we finally have,

$$
\begin{aligned}
y_{i+1} = y_{1,i+1} &= y_{1,i} + \frac{1}{6}(k_{1,1} + 2k_{2,1} + 2k_{3,1} + k_{4,1}) && (21)\\
z_{i+1} = y_{2,i+1} &= y_{2,i} + \frac{1}{6}(k_{1,2} + 2k_{2,2} + 2k_{3,2} + k_{4,2}). && (22)
\end{aligned}
$$

Note that we must calculate

$k_{1,1},\ k_{1,2},\ k_{2,1},\ k_{2,2},\ k_{3,1},\ k_{3,2},\ k_{4,1},\ k_{4,2}$ in that order.

Converting an n^{th} Order ODE to a System of First Order ODEs

Consider the general second order IVP

$$y'' + ay' + by = 0, \quad y(0) = \alpha_1, \quad y'(0) = \alpha_2$$

If we let

$$z = y', \quad z' = y''$$

then the original ODE can now be written as

$$\begin{aligned} y' &= f(x,y,z) = z, \quad y(0) = \alpha_1 & (23) \\ z' &= g(x,y,z) = -az - by, \quad z(0) = \alpha_2 & (24) \end{aligned}$$

Once transformed into a system of first order ODEs the methods for systems of equations apply.
Remember the solution is only $y_1, y_2, y_3, \ldots$ and **not** $z_1, z_2, z_3, \ldots$ (why is that?)

Boundary value problems (BVPs)

A linear second order boundary value problem (BVP) is

$$\begin{cases} y''(x) + p(x)y'(x) + q(x)y(x) = r(x) \\ y(a) = \alpha, \qquad y(b) = \beta \end{cases}$$

and a nonlinear second order boundary value problem (BVP) is

$$\begin{cases} y''(x) = f(x, y'(x), y''(x)) \\ y(a) = \alpha, \qquad y(b) = \beta \end{cases}$$

Finite difference for (BVPs)

Here we solve only a linear second order BVP:

$$\begin{cases} y''(x) + p(x)y'(x) + q(x)y(x) = r(x) \\ y(a) = \alpha, \qquad y(b) = \beta \end{cases}$$

First subdivide $[a, b]$ into N subintervals with size h. So

$$h = \frac{b-a}{N}, \qquad x_i = a + ih, \quad i = 0, 1, \cdots, N.$$

The finite difference method for (BVPs) consists of replacing derivatives in the BVP by difference approximations. For example:

$$y'(x_i) \approx \frac{y(x_{i+1}) - y(x_{i-1})}{2h}$$

$$y''(x_i) \approx \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2}$$

Finite difference for (BVPs) ctd

Substituting these approximations in the BVP we get:

$$\left(1-\frac{h}{2}p_i\right)y_{i-1}+(-2+h^2q_i)y_i+\left(1+\frac{h}{2}p_i\right)y_{i+1}=h^2r_i, \quad (25)$$

where $i=1,2,\cdots,N-1, \quad y_0=\alpha, \quad y_N=\beta$ and

$$y_i \approx y(x_i), \quad p_i=p(x_i), \quad q_i=q(x_i), \quad r_i=r(x_i).$$

So there are $N-1$ equations in $N-1$ unknowns.

System of $N-1$ equations in $N-1$ unknowns

$$\begin{bmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & 0 & \\ & a_3 & b_3 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & & a_{n-1} & b_{n-1} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{N-2} \\ y_{N-1} \end{bmatrix} = \begin{bmatrix} d_1 - a_1\alpha \\ d_2 \\ d_3 \\ \vdots \\ d_{N-2} \\ d_{N-1} - c_{N-1}\beta \end{bmatrix},$$

where

$$a_i = 1 - \frac{h}{2}p_i, \quad b_i = -2 + h^2 q_i, \quad c_i = 1 + \frac{h}{2}p_i, \quad d_i = h^2 r_i,$$

for $i = 1, 2, \cdots, N-1$.
This is a tridiagonal system using Gaussian elimination, LU factorisation etc.

Example of BVP using difference approximations

Solve the second order BVP:

$$\begin{cases} y''(x) + (x+1)y'(x) - 2y(x) = (1-x^2)e^{-x} \\ y(0) = -1, \qquad y(1) = 0 \end{cases},$$

using $h = 0.2$. Compare the approximate solution with exact solution $y = (x-1)e^{-x}$.
Solution: Here

$$p(x) = (x+1), \quad q(x) = -2, \quad r(x) = (1-x^2)e^{-x}.$$

Equation (25) becomes

$$[1 - 0.1(x_i + 1)]y_{i-1} + (-2 - 0.08)y_i + [1 + 0.1(x_i + 1)]y_{i+1} \\ = 0.04(1 - x_i^2)e^{-x_i},$$

where $y_0 = -1, \quad y_5 = 0$ and $x_i = 0.2i, \quad i = 1, 2, 3, 4$

Example of BVP using difference approximations

The resulting system of equations is

$$\begin{bmatrix} -2.08 & 1.12 & 0 & 0 \\ 0.86 & -2.08 & 1.14 & 0 \\ 0 & 0.84 & -2.08 & 1.16 \\ 0 & 0 & 0.82 & -2.08 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 0.91143926 \\ 0.02252275 \\ 0.01404958 \\ 0.00647034 \end{bmatrix}$$

Comparison of exact and difference approximation

x	Difference solution	Exact solution
0.0	-1.00000000	-1.0000000
0.2	-0.65413043	-0.65498460
0.4	-0.40102860	-0.40219203
0.6	-0.21847768	-0.21952465
0.8	-0.08924136	-0.08986579
1.0	0.00000000	0.00000000