Adaptive Runge-Kutta Methods

MATH 375 *Numerical Analysis*

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Comparison of ODE Solvers

Suppose we wish to approximate the solution to the IVP:

$$y'(t) = f(t, y)$$
$$y(t_0) = y_0.$$

Let

$$k_1 = f(t_0, y_0)$$
$$k_2 = f\left(t_0 + \frac{h}{3}, y_0 + \frac{h}{3}k_1\right)$$
$$k_3 = f\left(t_0 + \frac{2h}{3}, y_0 + \frac{2h}{3}k_2\right)$$

then we may use either Heun's method or the open $n = 1$ N-C method.

Heun's Method

$$y(t_0+h) = y(t_0)+\frac{h}{4}(k_1+3k_3)+O(h^4)$$

Open $n = 1$ N-C Method

$$y(t_0+h) = y(t_0)+\frac{h}{2}(k_2+k_3)+O(h^3)$$

Numerical Difference Between Methods

Subtract the open $n = 1$ N-C method from Heun's method.

$$\begin{aligned} y(t_0+h) - y(t_0+h) &= y(t_0) + \frac{h}{4}(k_1 + 3k_3) + O(h^4) \\ &\quad - y(t_0) - \frac{h}{2}(k_2 + k_3) - O(h^3) \\ 0 &= \frac{h}{4}(k_1 - 2k_2 + k_3) + O(h^4) - O(h^3) \\ \frac{h}{4}(k_1 - 2k_2 + k_3) &= M\,h^3 + O(h^4) \end{aligned}$$

Remarks:

- M is a constant associated with the local truncation error of the open $n = 1$ N-C method.
- The error estimate can be used to adjust h to keep the error estimate smaller than some tolerance without making h too small.

Example

Consider the initial-value problem:

$$\frac{dy}{dt} = y - t^2 + 1$$
$$y(0) = \frac{1}{2}.$$

The exact solution is $y(t) = (1+t)^2 - \frac{1}{2}e^t$.

- We will use Heun's method to approximate $y(1)$ with an accuracy of 10^{-2}.
- There is no "best" way to choose the step size, so we pick $h = 0.5$.

Step 1

$$k_1 = f(t_0, y_0) = \frac{1}{2} - (0)^2 + 1 = 1.5$$

$$k_2 = f\left(t_0 + \frac{h}{3}, y_0 + \frac{h}{3}k_1\right) = f(0 + 0.5/3, 0.5 + 0.5(1.5)/3)$$

$$= 1.72222$$

$$k_3 = f\left(t_0 + \frac{2h}{3}, y_0 + \frac{2h}{3}k_2\right) = f(0 + 2(0.5)/3, 0.5 + 2(0.5)(1.72222)/3)$$

$$= 1.96296$$

Now check the expected accuracy of the calculation of $y(h) = y(0.5)$:

$$\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| = \left|\frac{0.5}{4}(1.5 - 2(1.72222) + 1.96296\right| \approx 0.002315 < 10^{-2}$$

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Since this is within the desired accuracy we may calculate

$$y(0.5) = y(0) + \frac{h}{4}(k_1 + 3k_3) = 0.5 + \frac{0.5}{4}(1.5 + 3(1.96296)) = 1.42361.$$

Step 2

$$
\begin{aligned}
k_1 &= f(0.5, 1.42361) = 2.17361 \\
k_2 &= f(0.5 + 0.5/3, 0.5 + 0.5(2.17361)/3) = 2.34144 \\
k_3 &= f(0.5 + 2(0.5)/3, 0.5 + 2(0.5)(2.34144)/3) = 2.50965
\end{aligned}
$$

Now check the expected accuracy of the calculation of $y(0.5 + h) = y(1.0)$:

$$
\begin{aligned}
\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| &= \left|\frac{0.5}{4}(2.17361 - 2(2.34144) + 2.50965\right| \\
&\approx 4.823 \times 10^{-5} < 10^{-2}
\end{aligned}
$$

Step 2

$$
\begin{aligned}
k_1 &= f(0.5, 1.42361) = 2.17361 \\
k_2 &= f(0.5 + 0.5/3, 0.5 + 0.5(2.17361)/3) = 2.34144 \\
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Now check the expected accuracy of the calculation of $y(0.5 + h) = y(1.0)$:

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\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| &= \left|\frac{0.5}{4}(2.17361 - 2(2.34144) + 2.50965\right| \\
&\approx 4.823 \times 10^{-5} < 10^{-2}
\end{aligned}
$$

Since this is within the desired accuracy we may calculate

$$
\begin{aligned}
y(1.0) = y(0.5) + \frac{h}{4}(k_1 + 3k_3) &= 1.42361 + \frac{0.5}{4}(2.17361 + 3(2.50965)) \\
&= 2.63643.
\end{aligned}
$$

Remarks

- Usually we do not know the exact value of the solution to an IVP, so the calculation of

$$\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right|$$

  provides an estimate of the accuracy.
- If the accuracy is larger than tolerance, then we may reduce the stepsize h and improve the accuracy.

Adjusting the Stepsize (1 of 2)

Suppose for a given h,

$$\left| \frac{h}{4}(k_1 - 2k_2 + k_3) \right| \approx M\,h^3 = K > \epsilon.$$

If q is "slightly" smaller than 1, a step of size $q\,h$ would produce an error of approximately $M(q\,h)^3$.

$$\begin{aligned} M(q\,h)^3 &< \epsilon \\ q^3(M\,h^3) &< \epsilon \\ q^3 K &< \epsilon \\ q &< \sqrt[3]{\frac{\epsilon}{K}} \end{aligned}$$

In general to be safe, we will adjust the stepsize by a factor of $\max\{0.9q, 0.1\}$.

Adjusting the Stepsize (2 of 2)

Suppose for a given h,

$$\left| \frac{h}{4}(k_1 - 2k_2 + k_3) \right| \approx M\,h^3 = K < \frac{1}{5}\epsilon.$$

Perhaps h could be increased while still keeping the error estimate smaller than ϵ. If q is close to 1, a step of size $q\,h$ would produce an error of approximately $M(q\,h)^3$.

$$\begin{aligned} M(q\,h)^3 &= \epsilon \\ q^3(M\,h^3) &= \epsilon \\ q^3 K &= \epsilon \\ q &= \sqrt[3]{\frac{\epsilon}{K}} > 1 \end{aligned}$$

In general to be safe, we will adjust the stepsize by a factor of $\min\{q, 5\}$.

Example (1 of)

Consider the IVP:

$$\frac{dy}{dt} = \frac{t^2 + y}{t - y^2}$$
$$y(0) = 5$$

We will approximate the solution to an accurary of $\epsilon = 10^{-4}$ and choose an initial $h = 0.5$.

Example (2 of)

With $h = 0.5$ and $\epsilon = 10^{-4}$,

$$
\begin{aligned}
k_1 &= -0.200000 \\
k_2 &= -0.203846 \\
k_3 &= -0.210204 \\
\left| \frac{h}{4}(k_1 - 2k_2 + k_3) \right| &= 3.14043 \times 10^{-4} > \epsilon
\end{aligned}
$$

Example (2 of)

With $h = 0.5$ and $\epsilon = 10^{-4}$,

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\begin{aligned}
k_1 &= -0.200000 \\
k_2 &= -0.203846 \\
k_3 &= -0.210204 \\
\left| \frac{h}{4}(k_1 - 2k_2 + k_3) \right| &= 3.14043 \times 10^{-4} > \epsilon \\
q = (0.9)\sqrt[3]{\frac{10^{-4}}{3.14043 \times 10^{-4}}} &= 0.614581.
\end{aligned}
$$

Example (3 of)

With $h = (0.5)(0.614581) = 0.307291$ and $\epsilon = 10^{-4}$,

$$\begin{aligned} k_1 &= -0.200000 \\ k_2 &= -0.202081 \\ k_3 &= -0.205085 \\ \left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| &= 7.09735 \times 10^{-5} < \epsilon \end{aligned}$$

Example (3 of)

With $h = (0.5)(0.614581) = 0.307291$ and $\epsilon = 10^{-4}$,

$$\begin{aligned} k_1 &= -0.200000 \\ k_2 &= -0.202081 \\ k_3 &= -0.205085 \\ \left| \frac{h}{4}(k_1 - 2k_2 + k_3) \right| &= 7.09735 \times 10^{-5} < \epsilon \\ y(h) = y(0) + \frac{h}{4}(k_1 + 3k_3) &= 4.93737 \end{aligned}$$

Example (4 of)

With $h = 0.307291$ and $\epsilon = 10^{-4}$,

$$
\begin{aligned}
k_1 &= -0.209046 \\
k_2 &= -0.213994 \\
k_3 &= -0.220010 \\
\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| &= 8.20966 \times 10^{-5} < \epsilon
\end{aligned}
$$

Example (4 of)

With $h = 0.307291$ and $\epsilon = 10^{-4}$,

$$
\begin{aligned}
k_1 &= -0.209046 \\
k_2 &= -0.213994 \\
k_3 &= -0.220010 \\
\left|\frac{h}{4}(k_1 - 2k_2 + k_3)\right| &= 8.20966 \times 10^{-5} < \epsilon \\
y(h) = y(0) + \frac{h}{4}(k_1 + 3k_3) &= 4.87061
\end{aligned}
$$

Example (5 of)

Example (6 of)

Example (7 of)

Example (8 of)

Homework

- Read Section $x.y$.
- Exercises: