Numerical solution of ODEs: multistage and predictor–corrector methods

Continuing with the idea of approximating the integral on the right-hand side of

$$u_{n+1} \approx u_n + \int_{t_n}^{t_{n+1}} f\big(t, u(t)\big)\, dt,$$

we can derive some further methods for computing approximate solution values $u_n \approx u(t_n)$ of

$$\frac{du}{dt} = f(t, u)$$

at a sequence of t-values $t_0,\ t_1,\ t_2,\ \ldots,\ t_N$, given that $u(t_0) = u_0$.

Midpoint method

If we approximate the integral $\int_{t_n}^{t_{n+1}} f\big(t, u(t)\big)\, dt$ by the *midpoint* rule, we get

$$u_{n+1} = u_n + h\, f\Big(t_n + \tfrac{h}{2},\ u\big(t_n + \tfrac{h}{2}\big)\Big)$$

Unfortunately, the $u\big(t_n + \frac{h}{2}\big)$ on the right-hand side is unknown, and since it does not also appear on the left-hand side, we cannot obtain either $u\big(t_n + \frac{h}{2}\big)$ or u_{n+1} by solving an equation as in the backward Euler or Crank–Nicolson cases.

To get around this problem, we *approximate* $u\big(t_n + \frac{h}{2}\big)$ with Euler's method, taking just a "half step" $\frac{h}{2}$ from t_n:

$$u\big(t_n + \tfrac{h}{2}\big) \approx u_n + \tfrac{h}{2}\, f(t_n, u_n)$$

Substituting this approximation into the previous formula gives the midpoint method, also called the "modified Euler" method:

$$u_{n+1} = u_n + h\, f\Big(t_n + \tfrac{h}{2},\ u_n + \tfrac{h}{2}\, f(t_n, u_n)\Big)$$

Note that this is an explicit method. It is also a so-called "two-stage" method because the algorithm involves computing two "slopes", with the first being fed into the second one:

$$s_1 = f(t_n,\ u_n) \quad \text{and} \quad s_2 = f\big(t_n + \tfrac{h}{2},\ u_n + \tfrac{h}{2}\, s_1\big).$$

Improved Euler (Heun) method

The Crank–Nicolson (trapezoidal) method

$$u_{n+1} = u_n + \frac{h}{2}\Big[f(t_n, u_n) + f(t_n + h,\ u_{n+1})\Big]$$

is implicit because the unknown u_{n+1} appears on both sides of the formula, but we can convert it to an explicit method if we replace the u_{n+1} in the right-hand side by its approximation obtained from Euler's method, namely $u_n + hf(t_n, u_n)$. The formula then becomes

$$u_{n+1} = u_n + \frac{h}{2}\Big[f(t_n, u_n) + f\big(t_n + h,\ u_n + hf(t_n, u_n)\big)\Big],$$

which is known as the "improved Euler" or Heun's method. This method again has two stages:

$$s_1 = f(t_n,\ u_n)$$
$$s_2 = f\big(t_n + h,\ u_n + h\, s_1\big)$$
$$\text{and then} \quad u_{n+1} = u_n + \frac{h}{2}\big[s_1 + s_2\big]$$

Heun's method is the simplest example of a **predictor–corrector method**, where an approximation generated by an *explicit* method (Euler's in this case), called the "predictor", replaces the unknown u_{n+1} in the right-hand side of an *implicit* formula (Crank–Nicolson method in this case), called the "corrector". The formula that results from such a substitution is explicit.

Four-stage Runge–Kutta method

Write $F(t) = f\big(t, u(t)\big)$. Approximating the integral $\displaystyle\int_{t_n}^{t_{n+1}} F(t)\,dt$ by *Simpson's* rule gives

$$\begin{aligned}\int_{t_n}^{t_{n+1}} F(t)\,dt &\approx \frac{1}{3}\cdot\frac{(t_{n+1}-t_n)}{2}\Big[F(t_n) + 4\,F\Big(\frac{t_n+t_{n+1}}{2}\Big) + F(t_{n+1})\Big] \\ &= \frac{h}{6}\Big[F(t_n) + 4\,F\Big(t_n+\frac{h}{2}\Big) + F(t_n+h)\Big]\end{aligned}$$

Then, approximate $F(t_n) = f\big(t_n, u(t_n)\big)$ by $f(t_n, u_n) \equiv s_1$.
Split the middle term $4\,F\big(t_n+\frac{h}{2}\big)$ into $2\,F\big(t_n+\frac{h}{2}\big) + 2\,F\big(t_n+\frac{h}{2}\big)$;
approximate the first two $F\big(t_n+\frac{h}{2}\big) = f\big(t_n+\frac{h}{2},\ u(t_n+\frac{h}{2})\big)$ by $f\big(t_n+\frac{h}{2},\ u_n+\frac{h}{2}\,s_1\big) \equiv s_2$;
approximate the second two $F\big(t_n+\frac{h}{2}\big) = f\big(t_n+\frac{h}{2},\ u(t_n+\frac{h}{2})\big)$ by $f\big(t_n+\frac{h}{2},\ u_n+\frac{h}{2}\,s_2\big) \equiv s_3$.
Finally, approximate $F(t_n+h) = f\big(t_n+h,\ u(t_n+h)\big)$ by $f(t_n+h,\ u_n+h\,s_3) \equiv s_4$.
The formula for the method is then

$$u_{n+1} = u_n + \frac{h}{6}\,\big[s_1 + 2s_2 + 2s_3 + s_4\big]$$

General Runge–Kutta methods

A general Runge–Kutta method with k stages is characterized by a set of parameters α_i, β_{ij} and γ_i for $i = 1, 2, \ldots, k$. The ith stage computes a slope s_i by evaluating f at a value of t in $[t_n, t_{n+1}]$ and a value of u obtained by adding to u_n a linear combination of the previously computed slopes:

$$s_i = f\Bigg(t_n + \alpha_i h,\ u_n + h\sum_{j=1}^{i-1}\beta_{ij}s_j\Bigg)$$

The next approximate solution value u_{n+1} is also computed by adding to u_n a linear combination of slopes:

$$u_{n+1} = u_n + h\sum_{i=1}^{k}\gamma_i s_i$$

Euler's method uses just one slope and overestimates or underestimates the true solution (depending on whether the solution curve is concave down or up); we can think of Runge–Kutta methods as attempts to improve upon Euler's method by calculating several "adjusted" slopes and then taking a weighted average of them.

The parameters defining a Runge–Kutta method are often presented in a "Butcher tableau"

$$\begin{array}{c|cccc} \alpha_1 & & & & \\ \alpha_2 & \beta_{21} & & & \\ \alpha_3 & \beta_{31} & \beta_{32} & & \\ \vdots & \vdots & & \ddots & \\ \alpha_k & \beta_{k1} & \cdots & \beta_{k,k-1} & \\ \hline & \gamma_1 & \cdots & \gamma_k & \end{array}$$

For example, the 4-stage method above is

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

and there are 3-stage methods given by

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ \frac{3}{4} & 0 & \frac{3}{4} & \\ \hline & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} \end{array}$$

The midpoint and Heun methods are both 2-stage Runge–Kutta methods.