Runge-Kutta Methods

Euler's method:

$$\begin{aligned}
t_{i+1} &= t_i, \\
y_{i+1} &= y_i + hy'(t_i) + \frac{h^2}{2} y^{(2)}(c_i), \\
&= y_i + hf(t_i, y_i) + \frac{h^2}{2} y^{(2)}(c_i), && \text{(exact solution)} \\
w_{i+1} &= w_i + hf(t_i, w_i). && \text{(approximate solution)}
\end{aligned}$$

Taylor's Method of Order 2:

$$\begin{aligned}
t_{i+1} &= t_i, \\
y_{i+1} &= y_i + hy'(t_i) + \frac{h^2}{2} y''(t_i) + \frac{h^3}{6} y^{(3)}(c_i), \\
&= y_i + hf(t_i, y_i) + \frac{h^2}{2}\left(\frac{\partial}{\partial t} f(t_i, y_i) + f(t_i, y_i)\frac{\partial}{\partial y} f(t_i, y_i)\right) + \frac{h^3}{6} y^{(3)}(c_i), && \text{(exact solution)} \quad (1) \\
w_{i+1} &= w_i + hf(t_i, w_i) + \frac{h^2}{2}\left(\frac{\partial}{\partial t} f(t_i, w_i) + f(t_i, w_i)\frac{\partial}{\partial y} f(t_i, w_i)\right). && \text{(approximate solution)}
\end{aligned}$$

Taylor's method of Order 2 has local truncation error $O(h^2)$, which makes it preferable to Euler's method, but requires the computation of the derivatives of f, which make it undesirable.

1. **Runge-Kutta methods** use the higher order local truncation error of the Taylor methods while eliminating the computation and evaluation of the derivatives of f.
2. As such, Runge-Kutta methods are very popular numerical ODE solvers.
3. A Runge-Kutta method of Order n will have local truncation error of $O(h^n)$.

Taylor's Theorem for two variables Suppose that $f(t, y)$ and all its partial derivatives of order less than or equal to $n+1$ are continuous on $D = \{(t, y) \mid a \le t \le b, -\infty < y < \infty\}$. Let $(t_0, y_0) \in D$. For every $(t, y) \in D$, there exists c between t and t_0 and η between y and y_0 such that

$$\begin{aligned}
f(t, y) &= P_n(t, y) + R_n(t, y), \\
P_n(t, y) &= f(t_0, y_0) + \left[(t - t_0)\frac{\partial f}{\partial t}(t_0, y_0) + (y - y_0)\frac{\partial f}{\partial y}(t_0, y_0)\right] \\
&\quad + \left[\frac{1}{2}(t - t_0)^2 \frac{\partial^2 f}{\partial t^2}(t_0, y_0) + (t - t_0)(y - y_0)\frac{\partial^2 f}{\partial t \partial y}(t_0, y_0) + \frac{1}{2}(y - y_0)^2 \frac{\partial^2 f}{\partial y^2}(t_0, y_0)\right] \\
&\quad + \cdots + \left[\frac{1}{n!}\sum_{j=0}^{n} \binom{n}{j} (t - t_0)^{n-j}(y - y_0)^j \frac{\partial^n f}{\partial t^{n-j} \partial y^j}(t_0, y_0)\right], \\
R_n(t, y) &= \frac{1}{(n+1)!}\sum_{j=0}^{n+1} \binom{n+1}{j} (t - t_0)^{n+1-j}(y - y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j} \partial y^j}(c, \eta).
\end{aligned}$$

Runge-Kutta Methods of Order 2

For Taylor's method of Order 2, we wish to replace the derivative $y''(t_i)$, which we obtain using the DE as $y''(t) = \frac{d}{dt} f(t, y)$. Here is how it is done–the manipulations are straightforward, albeit a bit tedious.

Expanding f in a Taylor series about (t_i, y_i) then evaluating at $t = t_i + \alpha_1$ and $y = y_i + \beta_1$, we have:

$$
\begin{aligned}
f(t_i + \alpha_1, y_i + \beta_1) &= f(t_i, y_i) + \left[\alpha_1 \frac{\partial f}{\partial t}(t_i, y_i) + \beta_1 \frac{\partial f}{\partial y}(t_i, y_i) \right] + R_1(t_i + \alpha_1, y_i + \beta_1), \qquad (2) \\
R_1(t_i + \alpha_1, y_i + \beta_1) &= \left[\frac{\alpha_1^2}{2} \frac{\partial^2 f}{\partial t^2}(c, \eta) + \alpha_1 \beta_1 \frac{\partial^2 f}{\partial t \partial y}(c, \eta) + \frac{\beta_1^2}{2} \frac{\partial^2 f}{\partial y^2}(c, \eta) \right],
\end{aligned}
$$

for some c between t_i and $t_i + \alpha_1$ and η between y_i and $y_i + \beta_1$.

Now, multiply Eq. (2) by the parameter a_1 (note this is a_1 not α_1):

$$
a_1 f(t_i + \alpha_1, y_i + \beta_1) = a_1 f(t_i, y_i) + \left[a_1 \alpha_1 \frac{\partial f}{\partial t}(t_i, y_i) + a_1 \beta_1 \frac{\partial f}{\partial y}(t_i, y_i) \right] + a_1 R_1(t_i + \alpha_1, y_i + \beta_1). \qquad (3)
$$

We want to use Eq. (3) to replace f in Eq. (1). Matching the coefficients of f and its derivatives, we get the following equations (neglecting the error term for the moment):

$$
\begin{aligned}
a_1 &= h, \\
a_1 \alpha_1 &= h^2/2, \\
a_1 \beta_1 &= h^2 f(t_i, y_i)/2,
\end{aligned}
$$

from which we can determine

$$
\begin{aligned}
a_1 &= h, \\
\alpha_1 &= h/2, \\
\beta_1 &= h f(t_i, y_i)/2.
\end{aligned}
$$

With these substitutions, we can say from (3)

$$
h f(t_i, y_i) + \frac{h^2}{2} \left(\frac{\partial}{\partial t} f(t_i, y_i) + f(t_i, y_i) \frac{\partial}{\partial y} f(t_i, y_i) \right) = h f \left(t_i + \frac{h}{2}, y_i + \frac{h}{2} f(t_i, y_i) \right),
$$

and we have a new method (the Midpoint Method):

$$
\begin{aligned}
w_0 &= y_0, \\
w_{i+1} &= w_i + h f \left(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i) \right),
\end{aligned}
$$

with error given by

$$
R_1(t_i + \alpha_1, y_i + \beta_1) = \frac{h^2}{8} \frac{\partial^2 f}{\partial t^2}(c, \eta) + \frac{h^2}{4} \frac{\partial^2 f}{\partial t \partial y}(c, \eta) + \frac{h^2}{2} \frac{\partial^2 f}{\partial y^2}(c, \eta).
$$

If all the second order partial derivatives are bounded, then R_1 will be $O(h^2)$, which makes the Midpoint method a Runge-Kutta Method of Order 2.

Any method that replaces the derivatives if f with functional evaluations of f is considered a Runge-Kutta method. We can make different substitutions and choices and arrive at different Runge-Kutta methods.

Other Runge-Kutta Order 2 Methods

Let's approach this in a slightly different manner than before. We can assume the approximation to f terms in Eq. (1) has a certain form, with certain unspecified parameters, and then the goal will be to determine the parameters.

For example, we can choose to match with the approximation:

$$\begin{aligned} y_i + hf(t_i, y_i) + \frac{h^2}{2}\left(\frac{\partial}{\partial t}f(t_i, y_i) + f(t_i, y_i)\frac{\partial}{\partial y}f(t_i, y_i)\right) &= y_i + a_1 k_1 + a_2 k_2, \\ k_1 &= hf(t_i, y_i), \\ k_2 &= hf(t_i + h\alpha_2, y_i + k_1\beta_2), \end{aligned}$$

where the parameters $a_1, a_2, \alpha_2, \beta_2$ need to be determined, and the k_1, k_2 were introduced to assist with the nesting in the second variable.

We proceed by expanding everything in powers of h, and then forcing coefficients of powers of h to be equal, this assuring the approximation is correct to $O(h^2)$. Since we have four unknowns, and are expanding to $O(h^2)$, we get three equations. The details of this process are in *Mathematica*, and the final result is:

$$\begin{aligned} a_1 &= 1 - a_2, \\ \alpha_2 &= \frac{1}{2a_2}, \\ \beta_2 &= \frac{1}{2a_2}. \end{aligned}$$

If we choose $a_2 = 1$ we get $a_1 = 0, \alpha_2 = \beta_2 = 1/2$ **(Midpoint Method)**:

$$\begin{aligned} t_{i+1} &= t_i + h, \\ k_2 &= hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}k_1), \\ w_{i+1} &= w_i + k_2. \end{aligned}$$

If we choose $a_2 = 1/2$ we get $a_1 = a_2 = 1/2, \alpha_2 = \beta_2 = 1$ **(Explicit Trapezoidal Method)**:

$$\begin{aligned} t_{i+1} &= t_i + h, \\ k_1 &= hf(t_i, w_i), \\ k_2 &= hf(t_i + h, w_i + k_1), \\ w_{i+1} &= w_i + \frac{1}{2}(k_1 + k_2). \end{aligned}$$

If we choose $a_2 = 3/4$ we get $a_1 = 1/4, \alpha_2 = \beta_2 = 2/3$ **(Heun's Method)**:

$$\begin{aligned} t_{i+1} &= t_i + h, \\ k_1 &= hf(t_i, w_i), \\ k_2 &= hf(t_i + \frac{2}{3}h, w_i + \frac{2}{3}k_1), \\ w_{i+1} &= w_i + \frac{1}{4}(k_1 + 3k_2). \end{aligned}$$

Runge-Kutta Order 4 (RK4)

The most commonly used Runge-Kutta method is of order 4. It can be derived in a manner similar to what we did for order 3, only the algebra becomes extremely tedious.

The RK4 method is easy to program, is a one-step method (so only needs an initial condition to get started), and is considerably more accurate than the order 2 methods.

$$
\begin{aligned}
t_{i+1} &= t_i + h, \\
k_1 &= hf(t_i, w_i), \\
k_2 &= hf(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_1), \\
k_3 &= hf(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_2), \\
k_4 &= hf(t_i, w_i + k_3), \\
w_{i+1} &= w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).
\end{aligned}
$$