Derivation of Runge-Kutta methods

First recall Taylor methods:

\[ y(t + k) = y + k y' + \frac{k^2}{2} y'' + \frac{k^3}{6} y''' + \ldots \quad \text{(where \ y', y'', etc. are evaluated at time \ t)} \]

\[ = y + kf + \frac{k^2}{2} f' + \frac{k^3}{6} f'' + \ldots \quad \text{Swap \ y' for f according to the ODE \ y'(t) = f(t, y(t))} \]

We next swap all derivatives \( f^{(k)} \) into partial derivatives \( f_x, f_y \) of \( f \):

\[ f'(t, y) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \frac{dy}{dt} = f_t + f_y \frac{dy}{dt} \]

Recall that \( y(t) \) is a function of \( t \), so need chain rule:

\[ f''(t, y) = \ldots = f_{y y} + f_y f'_y + f_f f_{y y} + 2 f_y f_{y y} + f_n \]

etc.

These chain rule expansions can be done conveniently in Mathematica:

In: \[ f[t, y[t]] \]

Out: \[ f[t, y[t]] \]

Tell that \( f \) is a function of \( t \) and \( y[t] \)

In: \[ D[%, t]/.y'[t]->f[t, y[t]] \]

Out: \[ f[t, y[t]] f^{(0,1)}[t, y[t]]+f^{(1,0)}[t, y[t]] \]

Differentiate previous output with respect to \( t \) and also substitute \( f \) for \( y' \)

In: \[ D[%, t]/.y'[t]->f[t, y[t]] \]

Out: \[ f[t, y[t]] f^{(0,1)}[t, y[t]]+f^{(1,0)}[t, y[t]]+f^{(0,1)}[t, y[t]]+f^{(1,1)}[t, y[t]]+f^{(0,2)}[t, y[t]] \]

etc.

Hence, the Taylor method of order 3 becomes

\[ y(t + k) = y + kf + \frac{k^2}{2} (f_t + f_y f'_y) + \frac{k^3}{6} (f_{y y} + f_{y y} f'_y + f_f f_{y y} + 2 f_y f_{y y} + f_n) \]

Derive Runge-Kutta methods:

First recall the explicit form of the simplest second order algorithm

<table>
<thead>
<tr>
<th>Butcher diagram</th>
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<tbody>
<tr>
<td>( d^{(1)} ) = ( k f(t + 0 \cdot k, y) )</td>
</tr>
<tr>
<td>( d^{(2)} ) = ( k f(t + 1 \cdot k, y + d^{(1)}) )</td>
</tr>
<tr>
<td>( y(t + k) = y(t) + \frac{1}{2} d^{(1)} + \frac{1}{2} d^{(2)} )</td>
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<td>( \frac{1}{2} )</td>
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To find the coefficients of a general RK method of order 2:

\[
\begin{align*}
\frac{\text{d}y(t+k)}{\text{d}t} &= \frac{y(t) + b_1 d_1^{(1)} + b_2 d_2^{(2)}}{b_1 + b_2} \\
\end{align*}
\]

we Taylor expand \(d_1^{(1)}\) and \(d_2^{(2)}\) to second order:

In: \(d_1 = \text{Series}[k \ f[t_,y[t_]],\{k,0,2\}]\)
Out: \(f[t_,y[t_]]k + O[k]^3\)

In: \(d_2 = \text{Series}[k \ f[t_+c k,y[t_]+a d_1],\{k,0,2\}]\)
Out: \(f[t_,y[t_]]k+(a f[t_,y[t_]] f^{(0,1)}{[t_,y[t_]]}+c f^{(1,0)}{[t_,y[t_]]})k^2 + O[k]^3\)

and the combine the two:

In: \(b_1 d_1 + b_2 d_2\)
Out: \((b_1 f[t_,y[t_]]+b_2 f[t_,y[t_]])k + \\
\qquad b_2(a f[t_,y[t_]] f^{(0,1)}{[t_,y[t_]]}+c f^{(1,0)}{[t_,y[t_]]})k^2 + O[k]^3\)

i.e. \(y(t+k) = y(t) + k(b_1 + b_2)f + k^2(b_2 c f_i + b_2 a f_j) + O(k^3)\)

For an arbitrary function \(f(t,y)\), this matches the Taylor method of the same order if and only if

\[
\begin{align*}
b_1 + b_2 &= 1 \\
b_2 c &= \frac{1}{\tau} \\
b_2 a &= \frac{1}{\tau}
\end{align*}
\]

We can choose \(b_1\) and \(b_2\) arbitrary, subject to \(b_1 + b_2 = 1\). The values for \(c\) and \(a\) then follow. The particular choice \(b_1 = b_2 = \frac{1}{\tau}\) gives the 2-stage second order method we first quoted.

This derivation procedure generalizes to RK methods of higher orders. For example, to generate 4-stage RK methods of order 4, we would start with

\[
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
c_1 & a_{11} & & & \\
c_2 & a_{21} & a_{22} & & \\
c_3 & a_{31} & a_{32} & a_{33} & \\
\hline
b_1 & b_2 & b_3 & b_4 & 
\end{array}
\]

and then follow the procedure above to 4th order of accuracy. This turns out to give 9 compatibility conditions in 13 unknowns. For higher still orders of accuracy, the number of compatibility conditions increases rapidly, making it impossible to find \(p\)-stage methods of order \(p\) for \(p > 4\). Furthermore, these (generally nonlinear) compatibility conditions become increasingly difficult to find solutions to.