Derivation of Runge-Kutta methods

First recall Taylor methods:

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

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

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

$$f'(t,y) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt} = f_t + f\ f_y \qquad \text{Recall that } y(t) \text{ is a function of } t\text{, so need chain rule:}$$

$$f''(t,y) = \ldots \quad = f\ f_y^2 + f^2 f_{yy} + f_t f_y + 2f\ f_{ty} + f_{tt}\,,$$

etc.

These chain rule expansions can be done conveniently in Mathematica:

In: `f[t,y[t]]` Tell that f is a function of t and $y[t]$
Out: `f[t,y[t]]`

In: `D[%,t]/.y'[t]->f[t,y[t]]` Differentiate previous output with respect to t and also substitute f for y'
Out: `f[t,y[t]] f(0,1)[t,y[t]]+f(1,0)[t,y[t]]`

In: `D[%,t]/.y'[t]->f[t,y[t]]` Repeat the command from above.
Out:
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f(0,1)[t,y[t]](f[t,y[t]]f(0,1)[t,y[t]]+f(1,0)[t,y[t]])+ f[t,y[t]]f(1,1)[t,y[t]]+
f[t,y[t]](f[t,y[t]]f(0,2)[t,y[t]]+f(1,1)[t,y[t]])+f(2,0)[t,y[t]]
```
etc.

Hence, the Taylor method of order 3 becomes

$$y(t+k) = y + k\,f + \frac{k^2}{2}(f_t + f\ f_y) + \frac{k^3}{6}(f\ f_y^2 + f^2 f_{yy} + f_t f_y + 2f\ f_{ty} + f_{tt})$$

Derive Runge-Kutta methods:

First recall the explicit form of the simplest second order algorithm

$$\begin{aligned} d^{(1)} &= k\ f(t + 0\cdot k, y) \\ d^{(2)} &= k\ f(t + 1\cdot k, y + d^{(1)}) \\ \hline y(t+k) &= y(t) + \tfrac{1}{2}d^{(1)} + \tfrac{1}{2}d^{(2)} \end{aligned}$$

Butcher diagram

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \tfrac{1}{2} & \tfrac{1}{2} \end{array}$$

To find the coefficients of a general RK method of order 2:

$$\begin{array}{ll} d^{(1)} & = k\, f(t+0\cdot k, y) \\ d^{(2)} & = k\, f(t+c_1\cdot k, y+ad^{(1)}) \\ \hline y(t+k) & = y(t)+b_1 d^{(1)}+b_2 d^{(2)} \end{array}$$

$$\begin{array}{c|cc} 0 & & \\ c & a & \\ \hline & b_1 & b_2 \end{array}$$

we Taylor expand $d^{(1)}$ and $d^{(2)}$ to second order:

In: `d1 = Series[k f[t_,y[t_]],{k,0,2}]`
Out: `f[t_,y[t_]]k + O[k]³`

In: `d2 = Series[k f[t_+c k,y[t_]+a d1],{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_]])k² + O[k]³`

and the combine the two:

In: `b1 d1 +b2 d2`
Out: `(b1 f[t_,y[t_]]+b2 f[t_,y[t_]])k +`
`b2(a f[t_,y[t_]] f⁽⁰,¹⁾[t_,y[t_]]+c f⁽¹,⁰⁾[t_,y[t_]])k² + O[k]³`

i.e.

$$y(t+k) = y(t) + k(b_1+b_2)\, f + k^2(b_2 c\, f_t + b_2 a\, f\, f_y) + O(k^3)$$

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

$$\begin{cases} b_1 + b_2 & = 1 \\ b_2 c & = \frac{1}{2} \\ b_2 a & = \frac{1}{2} \end{cases}$$

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 $b_1 = b_2 = \frac{1}{2}$ 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

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

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.