Numerical Methods (See, *e.g.*, *Mathematical Methods of Physics*, by Mathews & Walker, *Computational Physics*, by Koonin, and *Numerical Recipes* by Press)

Imagine, as is often the case, that we know that the derivative of a function is given in terms of another function(al) of the original function and the free variable, e.g.,

$$\dot{y}(t) = f(t, y). \tag{NM.1}$$

We also know that $y(t_0) = y_0$ and we want to use this information to (numerically) find y at other values of t, *i.e.*, numerically solve the above equation. Previously we have considered cases where there is no t dependence on the right-hand-side and proceeded by separating variables and writing

$$dt = \frac{dy}{f(y)} \Rightarrow t - t_0 = \int_{y_0}^{y} \frac{dy'}{f(y')}. \tag{NM.2}$$

Even in this case we may not be able to perform the integral analytically and want to use numerical methods. A common method for numerically estimating an integral is to use Simpson's rule. Suppose we want to evaluate

$$I = \int_a^b f(x)dx, \tag{NM.3}$$

with $f(x)$ a known (but presumably complicated) function. Simpson says that we should divide the interval $\Delta x = b - a$ into n (n = even) smaller equal intervals, $h = \Delta x / n$ and calculate

$$\begin{aligned} I \simeq \frac{h}{3}\Big[& f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + 2f(a+4h) \\ & + \ldots + 2f(b-2h) + 4f(b-h) + f(b)\Big]. \end{aligned} \tag{NM.4}$$

We could apply this method above to find the time to go from y_0 to y_1, *i.e.*, $h = (y_1 - y_0)/n$. Using such a method one can test the reliability of the result by looking at how rapidly the numerical result varies as n is varied. Clearly one expects arbitrarily accurate results as $n \to \infty$.

Returning to the original problem, Eq. (NM.1), a typical approach would be to use the Runge-Kutta method. By using Taylor series expansion we can show that a good estimate of $y(t_0 + \delta)$ (to order δ^5) is provided by

$$
\begin{aligned}
&y(t_0 + \delta) \simeq y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\left[+O\left(\delta^5\right)\right], \\
&k_1 = \delta\, f\,(t_0, y_0), \\
&k_2 = \delta\, f\left(t_0 + \frac{\delta}{2}, y_0 + \frac{k_1}{2}\right), \\
&k_3 = \delta\, f\left(t_0 + \frac{\delta}{2}, y_0 + \frac{k_2}{2}\right), \\
&k_4 = \delta\, f\,(t_0 + \delta, y_0 + k_3).
\end{aligned}
\tag{NM.5}
$$

This result is, in fact quite similar to the Simpson result. To see where this comes from we define $f_0 = f\,(t_0, y_0)$, $f_0' = \partial f / \partial y\big|_{(t_0, y_0)}$, $\dot{f}_0 = \partial f / \partial t\big|_{(t_0, y_0)}$, *etc*. With this notation we can expand the above expressions (in general to arbitrary order, but here to order δ^4)

$$
\begin{aligned}
k_1 &= \delta f_0, \\
k_2 &\simeq \delta \left[f_0 + \frac{\delta}{2}\dot{f}_0 + \frac{k_1}{2} f_0' + \frac{\delta^2}{4\cdot 2}\ddot{f}_0 + 2\frac{\delta k_1}{4\cdot 2}\dot{f}_0' + \frac{k_1^2}{4\cdot 2} f_0'' \right. \\
&\qquad \left. + \frac{\delta^3}{8\cdot 6}\dddot{f}_0 + \frac{3}{8\cdot 6}\delta^2 k_1 \ddot{f}_0' + \frac{3}{8\cdot 6}\delta k_1^2 \dot{f}_0'' + \frac{k_1^3}{8\cdot 6} f_0''' \right] + O\left(\delta^5\right) \\
&= \delta \left[f_0 + \frac{\delta}{2}\dot{f}_0 + \frac{\delta}{2} f_0 f_0' + \frac{\delta^2}{8}\ddot{f}_0 + \frac{\delta^2}{4} f_0 \dot{f}_0' + \frac{\delta^2}{8} f_0^2 f_0'' \right. \\
&\qquad \left. + \frac{\delta^3}{48}\dddot{f}_0 + \frac{1}{16}\delta^3 f_0 \ddot{f}_0' + \frac{1}{16}\delta^3 f_0^2 \dot{f}_0'' + \frac{\delta^3}{48} f_0^3 f_0''' \right] + O\left(\delta^5\right), \\
&= \delta f_0 + \frac{\delta^2}{2}\left(\dot{f}_0 + f_0 f_0' \right) + \frac{\delta^3}{8}\left(\ddot{f}_0 + 2 f_0 \dot{f}_0' + f_0^2 f_0'' \right) \\
&\qquad + \frac{\delta^4}{48}\left(\dddot{f}_0 + 3 f_0 \ddot{f}_0' + 3 f_0^2 \dot{f}_0'' + f_0^3 f''' \right) + O\left(\delta^5\right),
\end{aligned}
\tag{NM.6}
$$

$$
\begin{aligned}
k_3 \simeq \delta \Bigg[& f_0 + \frac{\delta}{2} \dot{f}_0 + \frac{k_2}{2} f_0' + \frac{\delta^2}{4 \cdot 2} \ddot{f}_0 + 2 \frac{\delta k_2}{4 \cdot 2} \dot{f}_0' + \frac{k_2^2}{4 \cdot 2} f_0'' \\
& + \frac{\delta^3}{8 \cdot 6} \dddot{f}_0 + \frac{3}{8 \cdot 6} \delta^2 k_2 \ddot{f}_0' + \frac{3}{8 \cdot 6} \delta k_2^2 \dot{f}_0'' + \frac{k_2^3}{8 \cdot 6} f_0''' \Bigg] + O\left(\delta^5\right) \\
= \delta \Bigg[& f_0 + \frac{\delta}{2} \dot{f}_0 + \frac{1}{2} \left\{ \delta f_0 + \frac{\delta^2}{2} \left(\dot{f}_0 + f_0 f_0' \right) + \frac{\delta^3}{8} \left(\ddot{f}_0 + 2 f_0 \dot{f}_0' + f_0^2 f_0'' \right) \right\} f_0' \\
& + \frac{\delta^2}{8} \ddot{f}_0 + \frac{\delta}{4} \left\{ \delta f_0 + \frac{\delta^2}{2} \left(\dot{f}_0 + f_0 f_0' \right) \right\} \dot{f}_0' + \frac{1}{8} \left\{ \delta f_0 + \frac{\delta^2}{2} \left(\dot{f}_0 + f_0 f_0' \right) \right\}^2 f_0'' \\
& + \frac{\delta^3}{48} \dddot{f}_0 + \frac{1}{16} \delta^2 \left\{ \delta f_0 \right\} \ddot{f}_0' + \frac{1}{16} \delta \left\{ \delta f_0 \right\}^2 \dot{f}_0'' + \frac{\delta^3}{48} f_0^3 f_0''' \Bigg] + O\left(\delta^5\right), \\
= \delta f_0 & + \frac{\delta^2}{2} \left(\dot{f}_0 + f_0 f_0' \right) + \frac{\delta^3}{8} \left\{ \ddot{f}_0 + 2 f_0 \dot{f}_0' + 2 \left(\dot{f}_0 + f_0 f_0' \right) f_0' + f_0^2 f_0'' \right\} \\
+ \frac{\delta^4}{16} & \Big\{ \ddot{f}_0 f_0' + 4 f_0 f_0' \dot{f}_0' + 3 f_0^2 f_0' f'' + 2 \dot{f}_0 \dot{f}_0' + 2 f_0 \dot{f}_0 f_0'' \\
+ \frac{1}{3} & \dddot{f}_0 + f_0 \ddot{f}_0' + f_0^2 \dot{f}_0'' + \frac{1}{3} f_0^3 f_0''' \Big\} + O\left(\delta^5\right), \qquad \text{(NM.7)}
\end{aligned}
$$

$$k_4 \simeq \delta\left[f_0 + \delta\,\dot f_0 + k_3\, f_0' + \frac{\delta^2}{2}\,\ddot f_0 + 2\,\frac{\delta k_3}{2}\,\dot f_0' + \frac{k_3^2}{2}\,f_0'' \right.$$

$$\left. + \frac{\delta^3}{6}\,\dddot f_0 + \frac{3}{6}\delta^2 k_3\,\ddot f_0' + \frac{3}{6}\delta k_3^2\,\dot f_0'' + \frac{k_3^3}{6}\,f_0''' \right] + O\left(\delta^5\right)$$

$$= \delta\left[f_0 + \delta\,\dot f_0 + \left(\delta\, f_0 + \frac{\delta^2}{2}\left(\dot f_0 + f_0\, f_0' \right) \right.\right.$$

$$\left. + \frac{\delta^3}{8}\left\{ \ddot f_0 + 2\, f_0\, \dot f_0' + 2\left(\dot f_0 + f_0\, f_0' \right) f_0' + f_0^2\, f_0'' \right\} \right) f_0'$$

$$+ \frac{\delta^2}{2}\,\ddot f_0 + \delta\left(\delta\, f_0 + \frac{\delta^2}{2}\left(\dot f_0 + f_0\, f_0' \right) \right) \dot f_0' + \frac{\left(\delta\, f_0 + \frac{\delta^2}{2}\left(\dot f_0 + f_0\, f_0' \right) \right)^2}{2}\, f_0''$$

$$\left. + \frac{\delta^3}{6}\,\dddot f_0 + \frac{\delta^2}{2}(\delta\, f_0)\,\ddot f_0' + \frac{\delta}{2}(\delta\, f_0)^2\;\dot f_0'' + \frac{(\delta\, f_0)^3}{6}\, f_0''' \right] + O\left(\delta^5\right)$$

$$= \delta\, f_0 + \delta^2\left(\dot f_0 + f_0\, f_0' \right) + \frac{\delta^3}{2}\left\{ \dot f_0\, f_0' + f_0\left(f_0' \right)^2 + \ddot f_0 + 2\, f_0\, \dot f\,' + f_0^2\, f_0'' \right\}$$

$$+ \frac{\delta^4}{8}\left(\ddot f_0\, f_0' + 6\, f_0\, \dot f_0' f_0' + 2\left(\dot f_0\left(f_0' \right)^2 + f_0\left(f_0' \right)^3 \right) + 5\, f_0^2\, f_0' f_0'' + 4\,\dot f_0\, \dot f_0' \right.$$

$$\left. + 4\, f_0\, \dot f_0\, f_0'' + \frac{4}{3}\,\dddot f_0 + 4\, f_0\, \ddot f_0' + 4\, f_0^2\, \dot f_0'' + \frac{4}{3}\, f_0^3\, f_0''' \right) + O\left(\delta^5\right). \qquad \text{(NM.8)}$$

Thus, if we take the Runge-Kutta combination for the change in the function, we have

$$\frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4 \right) = \delta\, f_0 + \frac{\delta^2}{2}\left(\dot f_0 + f_0\, f_0' \right)$$

$$+ \frac{\delta^3}{6}\left(\ddot f_0 + 2\, f_0\, \dot f_0' + f_0\left(f_0' \right)^2 + \dot f_0\, f_0' + f_0^2\, f_0'' \right)$$

$$+ \frac{\delta^4}{24}\left(\dddot f_0 + \ddot f_0\, f_0' + 3\, f_0\, \ddot f_0' + 3\,\dot f_0\, \dot f_0' + 5\, f_0\, f_0' \dot f_0' + 3\, f_0^2\, \dot f_0'' \right. \qquad \text{(NM.9)}$$

$$\left. + 3\, f_0\, \dot f_0\, f_0'' + \dot f_0\left(f_0' \right)^2 + 4\, f_0^2\, \dot f_0\, f_0'' + f_0\left(f_0' \right)^3 + f_0^3\, f_0''' \right).$$

On the other hand we find by (tediously) taking derivatives directly

$$
\begin{aligned}
\dot{y}(t_0) &= f_0, \\
\ddot{y}(t_0) &= \dot{f}_0 + f_0 f_0', \\
\dddot{y}(t_0) &= \ddot{f}_0 + 2 f_0 \dot{f}_0' + f_0 \left(f_0' \right)^2 + \dot{f}_0 f_0' + f_0^{\,2} f_0'', \\
\ddddot{y}(t_0) &= \dddot{f}_0 + \ddot{f}_0 f_0' + 3 f_0 \ddot{f}_0' + 3 \dot{f}_0 \dot{f}_0' + 5 f_0 f_0' \dot{f}_0' + 3 f_0^{\,2} \dot{f}_0'' \\
&\quad + 3 f_0 \dot{f}_0 f_0'' + \dot{f}_0 \left(f_0' \right)^2 + 4 f_0^{\,2} \dot{f}_0 f_0'' + f_0 \left(f_0' \right)^3 + f_0^{\,3} f_0'''.
\end{aligned}
\qquad \text{(NM.10)}
$$

Thus, as advertised, the Runge-Kutta expression is the appropriate expansion, *i.e.*, the Taylor series. Clearly the Runge-Kutta notation is much more compact!