Difficulties with fixed-h Euler

- The low order results in requiring a small stepsize, which leads to a large number of derivative evaluations and excessive amount of computer time.
- The use of a constant stepsize can be inappropriate if the solution behaves differently on parts of the interval of interest. For example in integrating satellite orbits 'close approaches' typically requires a smaller stepsize to ensure accuracy.

Runge-Kutta Methods

We will consider a general class of one-step formulas of the form:

(1) $$y_j = y_{j-1} + h\Phi(x_{j-1}, y_{j-1}).$$

where Φ satisfies a Lipschitz condition with respect to y. That is,

$$|\Phi(x, u) - \Phi(x, v)| \le \mathcal{L}|u - v|.$$

We will consider a variety of choices for Φ and will observe that, in each case considered, Φ will be Lipschitz if f is.
Two examples of such formulas are:

Euler: $\Phi \equiv f$.

Taylor Series: $\Phi \equiv T_k(x, y)$.

Some Notation/Definitions

Definition: A formula (1) is of order p if for all sufficiently differentiable functions $y(x)$ we have,

(2) $$y(x_j) - y(x_{j-1}) - h\Phi(x_{j-1}, y(x_{j-1})) = O(h^{p+1}).$$

Note that:

1. The LHS of (2) is defined to be the Local Truncatiom Error (LTE) of the formula.

2. Order p implies that both the LE and the LTE are $O(h^{p+1})$. (This follows by substituting $z_j(x)$ for $y(x)$ in the definition.)

Main Result:

Theorem: A p^{th} order formula applied to an IVP with constant stepsize h satisfies,

$$|y(x_j) - y_j| \leq |e_0| e^{\mathcal{L}(b-a)} + \frac{Ch^p}{\mathcal{L}}(e^{\mathcal{L}(b-a)} - 1).$$

Runge-Kutta Methods (cont)

We wish to consider formulas Φ that are less 'expensive' than higher order Taylor Series and yet are higher order than Euler's formula. Consider a formula Φ based on 2 derivative evaluations. That is,

$$\Phi(x_{j-1}, y_{j-1}) = \omega_1 k_1 + \omega_2 k_2,$$

where,

$$\begin{aligned} k_1 &= f(x_{j-1}, y_{j-1}), \\ k_2 &= f(x_{j-1} + \alpha h, y_{j-1} + h\beta k_1). \end{aligned}$$

We determine the parameters $\omega_1, \omega_2, \alpha, \beta$ to obtain as high an order formula as possible.

RK Methods (cont)

From the definition of order we have order p if

(3) $$y(x_j) = y(x_{j-1}) \ + \ h(\omega_1 k_1 \ + \ \omega_2 k_2) \ + \ O(h^{p\,+\,1})$$

for all suff diff functions $y(x)$. To derive such a formula we expand $y(x_j), k_1, k_2$ in Taylor Series about the point (x_{j-1}, y_{j-1}), equate like powers of h on both sides of (3), and set $\alpha, \beta, \omega_1, \omega_2$ accordingly.

In what follows we omit arguments when they are evaluated at the point (x_{j-1}, y_{j-1}). The TS expansion of the LHS of (3) is:

$$\begin{aligned} y(x_j) &= y(x_{j-1}) + hy^{'}(x_{j-1}) + \frac{h^2}{2}y^{''}(x_{j-1}) + \frac{h^3}{6}y^{'''}(x_{j-1}) + O(h^4), \\ &= y(x_{j-1}) + hf + \frac{h^2}{2}(f_x + f_y f) \\ &\quad + \frac{h^3}{6}(f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y f_x + f_y^2 f) + O(h^4). \end{aligned}$$

Expansion of the RHS

The TS expansion of the RHS of (3) is more complicated and first requires the expansions of k_1 and k_2,

$$
\begin{aligned}
k_1 &= f, \\
k_2 &= f(x_{j-1} + \alpha h, y(x_{j-1}) + \beta h k_1), \\
&= f(x_{j-1}, y(x_{j-1}) + \beta h f) + (\alpha h) f_x(x_{j-1}, y(x_{j-1}) + \beta h f) \\
&\quad + \frac{\alpha^2 h^2}{2} f_{xx}(x_{j-1}, y(x_{j-1}) + \beta h f) + O(h^3), \\
&= \left[f + \beta h f f_y + \frac{(\beta h f)^2}{2} f_{yy} + O(h^3) \right] \\
&\quad + \left[\alpha h f_x + \alpha \beta h^2 f f_{xy} + O(h^3) \right] + \left[\frac{\alpha^2 h^2}{2} f_{xx} + O(h^3) \right], \\
&= f + (\beta f f_y + \alpha f_x) h + (\frac{\beta^2}{2} f^2 f_{yy} + \alpha \beta f f_{xy} + \frac{\alpha^2}{2} f_{xx}) h^2 + O(h^3).
\end{aligned}
$$

TS Expansion of the RHS

The TS expansion of the RHS of (3) then is (with these substitutions for k_1 and k_2)

$$
\begin{aligned}
RHS &= y(x_{j-1}) + h(\omega_1 k_1 + \omega_2 k_2), \\
&= y(x_{j-1}) + h\omega_1 f + h\omega_2 \left[\cdots\right] + O(h^4), \\
&= y(x_{j-1}) + \left[(\omega_1 + \omega_2) f\right] h + \left[\omega_2(\beta f f_y + \alpha f_x)\right] h^2 \\
&\quad + \left[\omega_2 (\frac{\beta^2}{2} f^2 f_{yy} + \alpha\beta f f_{xy} + \frac{\alpha^2}{2} f_{xx})\right] h^3 + O(h^4).
\end{aligned}
$$

and recall

$$
\begin{aligned}
LHS &= y(x_{j-1}) + hf + \frac{h^2}{2}(f_x + f_y f) \\
&\quad + \frac{h^3}{6}(f_{xx} + 2 f_{xy} f + f_{yy} f^2 + f_y f_x + f_y^2 f) + O(h^4).
\end{aligned}
$$

Equating like powers of h

Equating powers of h for LHS and RHS we observe:

For order 0 : The coefficients of h^0 always agree and we have order at least zero for any choice of the parameters.

For order 1: If $\omega_1 + \omega_2 = 1$ the coefficients of h^1 agree and we have at least order 1.

For order 2: In addition to satisfying the order 1 constraints we must have the coefficient of h^2 the same. That is $\alpha\omega_2 = 1/2$ and $\beta\omega_2 = 1/2$.

For order 3: In addition to satisfying the order 2 constraints we must have the coefficients of h^3 the same. That is we must satisfy the equations, $\omega_2\alpha^2 = \frac{1}{3}$, $\omega_2\alpha\beta = \frac{1}{3}$, $\omega_2\beta^2 = \frac{1}{3}$, $\frac{1}{6}f_{xy} = ?$, $\frac{1}{6}f_y^2 = ?$.

Family of 2^{nd}-order RK Formula

Note that there are not enough terms in the coefficient of h^3 in the expansion of the RHS to match the expansion of the LHS. We cannot therefore equate the coefficients of h^3 and the maximum order we can obtain is order 2. Our formula will be order 2 for any choice of $\omega_2 \neq 0$, with $\omega_1 = 1 - \omega_2$ and $\alpha = \beta = \frac{1}{2\omega_2}$. This is a one-parameter family of 2^{nd}-order Runge-Kutta formulas.

Three popular choices from this family are:

Modified Euler: $\omega_2 = 1/2$

$$
\begin{aligned}
k_1 &= f(x_{j-1}, y_{j-1}), \\
k_2 &= f(x_{j-1} + h, y_{j-1} + hk_1), \\
y_j &= y_{j-1} + \frac{h}{2}(k_1 + k_2).
\end{aligned}
$$

Family of 2^{nd}-order RK Formula

Midpoint: $\omega_2 = 1$

$$\begin{aligned} k_1 &= f(x_{j-1}, y_{j-1}), \\ k_2 &= f(x_{j-1} + \frac{h}{2}, y_{j-1} + \frac{h}{2} k_1), \\ y_j &= y_{j-1} + h k_2. \end{aligned}$$

Heun's Formula: $\omega_2 = 3/4$

$$\begin{aligned} k_1 &= f(x_{j-1}, y_{j-1}), \\ k_2 &= f(x_{j-1} + \frac{2}{3} h, y_{j-1} + \frac{2}{3} h k_1), \\ y_j &= y_{j-1} + \frac{h}{4}(k_1 + 3k_2). \end{aligned}$$

Higher-Order RK Formulas

An s-stage explicit Runge-Kutta formula uses s derivative evaluations and has the form:

$$y_j = y_{j-1} + h(\omega_1 k_1 + \omega_2 k_2 \cdots + \omega_s k_s),$$

where

$$\begin{aligned}
k_1 &= f(x_{j-1}, y_{j-1}), \\
k_2 &= f(x_{j-1} + \alpha_2 h, y_{j-1} + h\beta_{21} k_1), \\
\vdots & \qquad \vdots \\
k_s &= f(x_{j-1} + \alpha_s h, y_{j-1} + h \sum_{r=1}^{s-1} \beta_{sr} k_r).
\end{aligned}$$

Higher-Order RK Formulas (cont)

This formula is represented by the tableau,

$$
\begin{array}{c|cccccc}
- & - & & & & \\
\alpha_2 & \beta_{21} & - & & & \\
\vdots & \vdots & & & & \\
\alpha_s & \beta_{s1} & \beta_{s2} & \ldots & \beta_{s-1,s} & - \\
\hline
 & \omega_1 & \omega_2 & \ldots & & \omega_s
\end{array}
$$

These $\frac{s(s-1)}{2} + (s-1) + s$ parameters are usually chosen to maximise the order of the formula.

Higher-Order RK Formulas (cont)

The maximum attainable order for an s-stage Runge-Kutta formula is given by the following table:

s	1	2	3	4	5	6
max order	1	2	3	4	4	5

Note that the derivations of these maximal order formulas can be very messy and tedious, but essentially they follow (as outlined above for the case $s = 2$) by expanding each of the k_r in a Taylor series.

An Example – Runge's 4th order Formula(1895)

-	-			
1/2	1/2	-		
1/2	0	1/2	-	
1	0	0	1	-
	1/6	1/3	1/3	1/6

Error Estimates for RK Methods

- Ideally a method would estimate a bound on the global error and adjust the stepsize, h, to keep the magnitude of the global error less than a tolerance. Such computable bounds are possible but are usually pessimistic and inefficient to implement.
- On the other hand, local errors can be reliably controlled. Consider a method which keeps the magnitude of the local error less than $h\,TOL$ on each step.
  That is, if $z_j(x)$ is the local solution on step j,

  $$z_j^{'} = f(x, z_j),\ z_j(x_{j-1}) = y_{j-1},$$

  then a method will adjust $h = x_j - x_{j-1}$ to ensure that $|z_j(x_j) - y_j| \leq h\,TOL$, for $j = 1, 2 \cdots N_{TOL}$.