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,

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

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 $j = 1, 2 \cdots N_{TOL}$.

Error Control

With this type of error control one can show that, for the resulting approximate solution

$$(x_j, y_j)_{j=0}^{N_{TOL}}$$

there exists a piecewise polynomial, $Z(x) \in C^1[a, b]$ such that $Z(x_j) = y_j$ for $j = 0, 1, \cdots N_{TOL}$ and for $x \in [a, b]$,

$$|Z^{'}(x) - f(x, Z)| \leq TOL.$$

This inequality can be shown to imply,

$$|y(x_j) - y_j| \leq \frac{TOL}{L}(e^{L(x_j - a)} - 1).$$

Local Error Estimates

Consider the Modified Euler Formula:

-	-	
1	1	-
	1/2	1/2

We have shown

$$\begin{aligned} z_j(x_j) &= y_{j-1} + \frac{h}{2}(k_1 + k_2) \\ &+ \left[\frac{1}{4} f^2 f_{yy} + \frac{1}{2} f f_{xy} + \frac{1}{4} f_{xx} - y^{'''}(x_j)\right] h^3 + O(h^4), \\ &= y_j + \left[\frac{1}{12} f_{yy} f^2 + \frac{1}{6} f f_{xy} + \frac{1}{12} f_{xx} - \frac{1}{6} f_{xy} - \frac{1}{6} f_y^2 f\right] h^3 + O(h^4), \\ &\equiv y_j + c(f) h^3 + O(h^4). \end{aligned}$$

Local Error Estimates (cont)

It then follows that the local error, LE, satisfies

$$LE = c(f)h^3 + O(h^4),$$

where $c(f)$ is a complicated function of f. There are two general strategies for estimating this LE, – the use of "step halving" and the use of a 3^{rd} order "companion formula".

Step Halving

Let $\hat{y}_j$ be the approximation to $z_j(x_j)$ computed with two steps of size $h/2$. If $c(f)$ is almost constant the we can show

$$z_j(x_j) = \hat{y}_j + 2c(f)(\frac{h}{2})^3 + O(h^4)$$

and from above

$$z_j(x_j) = y_j + c(f)h^3 + O(h^4).$$

Therefore the local error associated with $\hat{y}_j$, $\widehat{LE}$, is

$$\widehat{LE} \quad = \quad 2c(f)(\frac{h}{2})^3 + O(h^4) \quad = \frac{-1}{3}(y_j - \hat{y}_j) + O(h^4).$$

The method could then compute $\hat{y}_j, y_j$ and accept $\hat{y}_j$ only if $\frac{1}{3}|y_j - \hat{y}_j| < h\, TOL$.

Note that this strategy requires five derivative evaluations on each step and assumes that each of the components of $c(f)$ is slowly varying.

3^{rd}-Order Companion Formula

To estimate the local error associated with the Modified Euler formula consider the use of a 3-stage, 3^{rd} order Runge-Kutta formula,

$$\hat{y}_j \quad = \quad y_{j-1} + h(\hat{\omega}_1 \hat{k}_1 + \hat{\omega}_2 \hat{k}_2 + \hat{\omega}_3 \hat{k}_3) \; = z_j(x_j) + O(h^4),$$

We also have

$$y_j \quad = \quad y_{j-1} + \frac{h}{2}(k_1 + k_2) \; = z_j(x_j) - c(f)h^3 + O(h^4).$$

Subtracting these two equations we have the local error estimate,

$$est_j \equiv (\hat{y}_j - y_j) = c(f)h^3 + O(h^4).$$

3^{rd}-Order Companion Formula

Note that, for any 3^{rd} order formula, $k_1 = \hat{k}_1$ and if $\hat{\alpha}_2 = \alpha_2 = 1$ and $\hat{\beta}_{21} = \beta_{21} = 1$, we have $\hat{k}_2 = k_2$ and the cost is only three derivative evaluations per step to compute both y_j and est_j. Can one derive such a 3-stage 3^{rd} order Runge-Kutta formula ? The following tableau with $\hat{\alpha}_3 \neq 1$ defines a one-parameter family of such "companion formulas" for Modified Euler:

-	-		
1	1	-	
$\hat{\alpha}_3$	$\hat{\beta}_{31}$	$\hat{\beta}_{32}$	-
	$\hat{\omega}_1$	$\hat{\omega}_2$	$\hat{\omega}_3$

with

$$\hat{\beta}_{31} = \hat{\alpha}_3^2,\ \hat{\beta}_{32} = \hat{\alpha}_3 - \hat{\alpha}_3^2,\ \hat{\omega}_2 = \frac{(3\hat{\alpha}_3 - 2)}{6(\hat{\alpha}_3 - 1)},\ \hat{\omega}_3 = \frac{-1}{6\hat{\alpha}_3(\hat{\alpha}_3 - 1)},\ \hat{\omega}_1 = \frac{13\hat{\alpha}_3 - 1}{6\hat{\alpha}_3}.$$

Higher-Order Companion Formulas

This idea of using a "companion formula" of order $p+1$ to estimate the local error of a p^{th} order formula leads to the derivation of s-stage, order $(p, p+1)$ formula pairs with the fewest number of stages. Such formula pairs can be characterized by the tableau:

-	-				
α_2	β_{21}	-			
$\vdots$	$\vdots$				
α_s	β_{s1}	$\dots$		$\beta_{s,s-1}$	-
	ω_1	ω_2	$\dots$		ω_s
	$\hat{\omega}_1$	$\hat{\omega}_2$	$\dots$		$\hat{\omega}_s$

Higher-Order Companion Formulas

Where

$$\begin{aligned} y_j &= y_{j-1} + h\sum_{r=1}^{s} \omega_r k_r &= z_j(x_j) - c(f)h^{p+1} + O(h^{p+2}), \\ \hat{y}_j &= y_{j-1} + h\sum_{r=1}^{s} \hat{\omega}_r k_r &= z_j(x_j) + O(h^{p+2}), \\ est_j &= (\hat{y}_j - y_j) &= c(f)h^{p+1} + O(h^{p+2}). \end{aligned}$$

This error estimate is a reliable estimate of the local error associated with the lower order (order p) formula. The following table gives the fewest number of stages required to generate formula pairs of a given order.

order pair	(2,3)	(3,4)	(4,5)	(5,6)	(6,7)
fewest stages	3	4	6	8	10

Choice of Stepsize, h

- Step is accepted only if $|est_j| < hTOL$.
- If h is too large, the step will be rejected.
- If h is too small, there will be too many steps.

The usual strategy for choosing the attempted stepsize, h, for the next step is based on 'aiming' at the largest h which will result in an accepted step on the current step. If we assume that $c(f)$ is slowly varying then,

$$|est_j| = |c(f)|h_j^{p+1} + O(h^{p+2}),$$

and on the next step attempted step, $h_{j+1} = \gamma h_j$, we want

$$|est_{j+1}| \approx TOL\ h_{j+1}.$$

Choice of h (cont)

But

$$|est_{j+1}| \approx |c(f)|(\gamma h_j)^{p+1} \quad = \gamma^{p+1}|est_j|.$$

We can then expect

$$|est_{j+1}| \approx TOL\ h_{j+1},$$

if

$$\gamma^{p+1}|est_j| \approx TOL\ (\gamma h_j),$$

which is equivalent to

$$\gamma^p|est_j| \approx TOL\ h_j.$$

Choice of h (cont)

The choice of γ to satisfy this heuristic is then,

$$\gamma = \left(\frac{TOL\, h_j}{|est_j|} \right)^{1/p}.$$

A typical step-choosing heuristic is then,

$$h_{j+1} = .9 \left(\frac{TOL\, h_j}{|est_j|} \right)^{1/p} h_j,$$

where $.9$ is a 'safety factor'. The formula works for use after a rejected step as well but must be modified slightly when round-off errors are significant (as might be the case for example when $TOL < 100\mu$).