Runge-Kutta methods

With orders of Taylor methods yet without derivatives of $f(t, y(t))$

First order Taylor expansion in two variables

Theorem: Suppose that $f(t, y)$ and all its partial derivatives are

continuous on $\quad D \overset{def}{=} \{(t, y) \,|\, \quad a \leq t \leq b, \quad c \leq y \leq d.\}$

Let $(t_0, y_0), (t, y) \in D, \Delta_t = t - t_0, \Delta_y = y - y_0$. **Then**

$$f(t, y) = P_1(t, y) + R_1(t, y), \quad \text{where}$$

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$$f(t,y) = P_1(t,y) + R_1(t,y), \quad \text{where}$$

$$\begin{aligned} P_1(t,y) &= f(t_0,y_0) + \Delta_t \frac{\partial f}{\partial t}(t_0,y_0) + \Delta_y \frac{\partial f}{\partial y}(t_0,y_0), \\ R_1(t,y) &= \frac{\Delta_t^2}{2}\frac{\partial^2 f}{\partial t^2}(\xi,\mu) + \Delta_t\,\Delta_y \frac{\partial^2 f}{\partial t \partial y}(\xi,\mu) + \frac{\Delta_y^2}{2}\frac{\partial^2 f}{\partial y^2}(\xi,\mu), \end{aligned}$$

for some point $(\xi, \mu) \in D$.

Second order Taylor expansion in two variables

Theorem: Suppose that $f(t, y)$ and all its partial derivatives are

$$\text{continuous on} \quad D \stackrel{def}{=} \{(t, y) \,|\quad a \leq t \leq b, \quad c \leq y \leq d.\}$$

Let $(t_0, y_0), (t, y) \in D, \Delta_t = t - t_0, \Delta_y = y - y_0$. **Then**

$$f(t, y) = P_2(t, y) + R_2(t, y), \quad \text{where}$$

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$$f(t, y) = P_2(t, y) + R_2(t, y), \quad \text{where}$$

$$\begin{aligned} P_2(t, y) \quad &= \quad f(t_0, y_0) + \left(\Delta_t \frac{\partial f}{\partial t}(t_0, y_0) + \Delta_y \frac{\partial f}{\partial y}(t_0, y_0)\right) \\ &+ \left(\frac{\Delta_t^2}{2} \frac{\partial^2 f}{\partial t^2}(t_0, y_0) + \Delta_t \, \Delta_y \frac{\partial^2 f}{\partial t \partial y}(t_0, y_0) + \frac{\Delta_y^2}{2} \frac{\partial^2 f}{\partial y^2}(t_0, y_0)\right), \end{aligned}$$

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Runge-Kutta Method of Order Two (III)

- **Midpoint Method**

$$
\begin{aligned}
w_0 &= \alpha, \\
w_{j+1} &= w_j + h\, f\left(t_j + \frac{h}{2}, w_j + \frac{h}{2} f(t_j, w_j)\right), \quad j = 0, 1, \cdots, N-1.
\end{aligned}
$$

- Two function evaluations for each j,
- Second order accuracy.

No need for derivative calculations

General 2nd order Runge-Kutta Methods

- $w_0 = \alpha$; for $j = 0, 1, \cdots, N-1$,

$$w_{j+1} = w_j + h\left(a_1 f(t_j, w_j) + a_2 f\left(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j)\right)\right).$$

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- Want to choose $a_1, a_2, \alpha_2, \delta_2$ for highest possible order of accuracy.

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- Two function evaluations for each j,
- Want to choose $a_1, a_2, \alpha_2, \delta_2$ for highest possible order of accuracy.

local truncation error

$$\begin{aligned}
\tau_{j+1}(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \left(a_1 f(t_j, y(t_j)) + a_2 f\left(t_j + \alpha_2, y(t_j) + \delta_2 f(t_j, y(t_j))\right)\right) \\
= \; y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\
- \Bigg((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2\, \frac{\partial f}{\partial t}(t_j, y(t_j)) \\
+ \; a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Bigg).
\end{aligned}$$

local truncation error

$$
\begin{aligned}
\tau_{j+1}(h) = \quad & y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\
& - \Bigg((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2\, \frac{\partial f}{\partial t}(t_j, y(t_j)) \\
& \qquad + \quad a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Bigg) .
\end{aligned}
$$

where $y'(t_j) = f(t_j, y(t_j))$,

local truncation error

$$\begin{aligned}\tau_{j+1}(h) = & \; y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\ & - \Big((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2 \frac{\partial f}{\partial t}(t_j, y(t_j)) \\ & \quad + \; a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Big) .\end{aligned}$$

where $y'(t_j) = f(t_j, y(t_j))$,

$$y''(t_j) = \frac{d\,f}{d\,t}(t_j, y(t_j)) = \frac{\partial f}{\partial t}(t_j, y(t_j)) + f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)).$$

For any choice with

$$a_1 + a_2 = 1, \quad a_2\, \alpha_2 = a_2\, \delta_2 = \frac{h}{2},$$

we have a second order method

$$\tau_{j+1}(h) = O(h^2).$$

local truncation error

$$\tau_{j+1}(h) = \quad y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2)$$
$$- \Bigg((a_1 + a_2)\, f(t_j, y(t_j)) + a_2\, \alpha_2\, \frac{\partial f}{\partial t}(t_j, y(t_j))$$
$$+ \quad a_2\, \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \Bigg) .$$

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we have a second order method

$$\tau_{j+1}(h) = O(h^2).$$

Four parameters, three equations

General 2nd order Runge-Kutta Methods

$w_0 = \alpha$; for $j = 0, 1, \cdots, N-1$,

$$w_{j+1} = w_j + h\left(a_1 f(t_j, w_j) + a_2 f\left(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j)\right)\right).$$

$$a_1 + a_2 = 1, \quad a_2\,\alpha_2 = a_2\,\delta_2 = \frac{h}{2},$$

- **Midpoint method**: $a_1 = 0, a_2 = 1, \alpha_2 = \delta_2 = \frac{h}{2}$,

$$w_{j+1} = w_j + h\,f\left(t_j + \frac{h}{2}, w_j + \frac{h}{2} f(t_j, w_j)\right).$$

- **Modified Euler method**: $a_1 = a_2 = \frac{1}{2}, \alpha_2 = \delta_2 = h$,

$$w_{j+1} = w_j + \frac{h}{2}\left(f(t_j, w_j) + f\left(t_{j+1}, w_j + hf(t_j, w_j)\right)\right).$$

3rd order Runge-Kutta Method (rarely used in practice)

$$w_0 = \alpha;$$
for $j = 0, 1, \cdots, N-1,$

$$w_{j+1} = w_j + \frac{h}{4}\left(f(t_j, w_j) + 3f\left(t_j + \frac{2h}{3}, w_j + \frac{2h}{3} f(t_j + \frac{h}{3}, w_j + \frac{h}{3} f(t_j, w_j))\right)\right)$$
$$\stackrel{def}{=} w_j + h\,\phi(t_j, w_j).$$

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$$\stackrel{def}{=} w_j + h\,\phi(t_j, w_j).$$

local truncation error

$$\tau_{j+1}(h) = \frac{y(t_{j+1}) y(t_j)}{h} - \phi(t_j, y(t_j)) = O(h^3).$$

4th order Runge-Kutta Method

$w_0 = \alpha;$
for $\quad j = 0, 1, \cdots, N-1,$

$$\begin{aligned}
k_1 &= h\, f(t_j, w_j), \\
k_2 &= h\, f\left(t_j + \frac{h}{2}, w_j + \frac{1}{2} k_1\right), \\
k_3 &= h\, f\left(t_j + \frac{h}{2}, w_j + \frac{1}{2} k_2\right), \\
k_4 &= h\, f\left(t_{j+1}, w_j + k_3\right), \\
w_{j+1} &= w_j + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right).
\end{aligned}$$

4 function evaluations per step

Example

Initial Value ODE	$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$
exact solution	$y(t) = (1 + t)^2 - 0.5\, e^t.$

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t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

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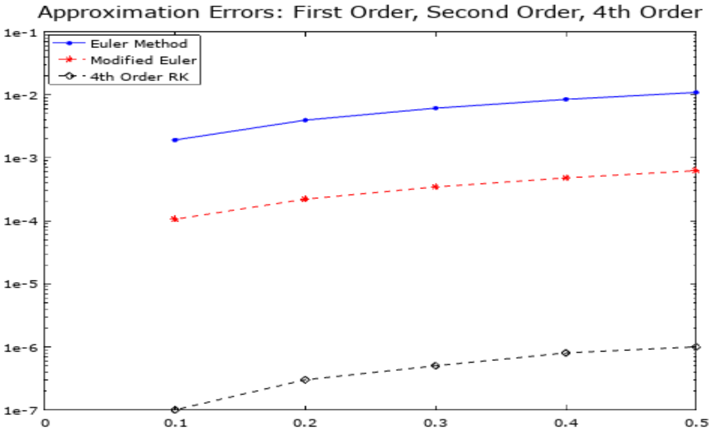

Adaptive Error Control (I)

$$\frac{dy}{dt} = f(t, y(t)), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

Consider a variable-step method with a well-chosen function $\phi(t, w, h)$:

- $w_0 = \alpha$.
- for $j = 0, 1, \cdots$,
  - **choose** step-size $h_j = t_{j+1} - t_j$,
  - **set** $w_{j+1} = w_j + h_j \, \phi\,(t_j, w_j, h_j)$.

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Adaptively choose step-size to satisfy given tolerance

Adaptive Error Control (II)

- Given an **order-n** method
  - $w_0 = \alpha$.
  - for $j = 0, 1, \cdots$,

$$w_{j+1} = w_j + h\,\phi\left(t_j, w_j, h\right), \quad h = t_{j+1} - t_j,$$

  - **local truncation error** (LTE)

$$\tau_{j+1}(h) = \frac{y(t_{j+1}) - y(t_j)}{h} - \phi\left(t_j, y(t_j), h\right) = O\left(h^n\right).$$

- Given tolerance $\tau > 0$, we would like to estimate **largest** step-size h for which

$$|\tau_{j+1}(h)| \lesssim \tau.$$

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Approach: Estimate $\tau_{j+1}(h)$ with **order-**$(n+1)$ method

$$\widetilde{w}_{j+1} = \widetilde{w}_j + h\,\widetilde{\phi}\,(t_j, \widetilde{w}_j, h)\,, \quad \text{for} \quad j \geq 0.$$

LTE Estimation (I)

- Assume $\quad w_j \approx y(t_j), \quad \widetilde{w}_j \approx y(t_j)$ (only estimating **LTE**).

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- $\phi(t, w, h)$ is order-n method

$$
\begin{aligned}
\tau_{j+1}(h) &\stackrel{def}{=} \frac{y(t_{j+1}) - y(t_j)}{h} - \phi\left(t_j, y(t_j), h\right) \\
&\stackrel{w_j \approx y(t_j)}{\approx} \frac{y(t_{j+1}) - \left(w_j + h\,\phi\left(t_j, w_j, h\right)\right)}{h} \\
&= \frac{y(t_{j+1}) - w_{j+1}}{h} = O\left(h^n\right).
\end{aligned}
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&= \frac{y(t_{j+1}) - w_{j+1}}{h} = O\left(h^n\right).
\end{aligned}
$$

- $\widetilde{\phi}(t, w, h)$ is order-$(n+1)$ method,

$$
\begin{aligned}
\widetilde{\tau}_{j+1}(h) &\stackrel{def}{=} \frac{y(t_{j+1}) - y(t_j)}{h} - \widetilde{\phi}\left(t_j, y(t_j), h\right) \\
&\stackrel{\widetilde{w}_j \approx y(t_j)}{\approx} \frac{y(t_{j+1}) - \left(\widetilde{w}_j + h\,\widetilde{\phi}\left(t_j, \widetilde{w}_j, h\right)\right)}{h} \\
&= \frac{y(t_{j+1}) - \widetilde{w}_{j+1}}{h} = O\left(h^{n+1}\right).
\end{aligned}
$$

LTE Estimation (III)

- Assume $\quad w_j \approx y(t_j), \quad \widetilde{w}_j \approx y(t_j) \quad$ (only estimating **LTE**).

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$$\tau_{j+1}(h) \quad \approx \quad \frac{y(t_{j+1}) - w_{j+1}}{h} = O\left(h^n\right).$$

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- $\widetilde{\phi}(t, w, h)$ is order-$(n+1)$ method,

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LTE Estimation (III)

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$$\widetilde{\tau}_{j+1}(h) \approx \frac{y(t_{j+1}) - \widetilde{w}_{j+1}}{h} = O\left(h^{n+1}\right).$$

- therefore

$$\begin{aligned}\tau_{j+1}(h) &\approx \frac{y(t_{j+1}) - \widetilde{w}_{j+1}}{h} + \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} \\ &= O\left(h^{n+1}\right) + \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} = O\left(h^n\right).\end{aligned}$$

LTE estimate: $\tau_{j+1}(h) \approx \dfrac{\widetilde{w}_{j+1} - w_{j+1}}{h}$

step-size selection (I)

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- Since $\tau_{j+1}(h) = O\left(h^n\right)$, **assume**

$$\tau_{j+1}(h) \approx K\, h^n \quad \text{where } K \text{ is independent of } h.$$

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$$\tau_{j+1}(h) \approx K\, h^n \quad \text{where } K \text{ is independent of } h.$$

- K should satisfy

$$K\, h^n \approx \frac{\widetilde{w}_{j+1} - w_{j+1}}{h}.$$

- **Assume** LTE for new step-size $q\,h$ satisfies given tolerance ϵ:

$$\left|\tau_{j+1}(q\,h)\right| \leq \epsilon, \quad \text{need to estimate } q.$$

step-size selection (II)

$$\text{LTE estimate: } K\,h^n \approx \tau_{j+1}(h) \approx \frac{\widetilde{w}_{j+1} - w_{j+1}}{h}$$

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$$\begin{aligned} |\tau_{j+1}(q\,h)| &\approx |K\,(q\,h)^n| = q^n\,|K\,h^n| \\ &\approx q^n \left| \frac{\widetilde{w}_{j+1} - w_{j+1}}{h} \right| \leq \epsilon. \end{aligned}$$

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$$\text{new step-size estimate: } q\,h \lesssim \left|\frac{\epsilon\,h}{\widetilde{w}_{j+1} - w_{j+1}}\right|^{\frac{1}{n}} h$$

Summary

- Given **order-**n method

$$w_{j+1} = w_j + h\,\phi\,(t_j, w_j, h)\,, \quad h = t_{j+1} - t_j, \quad j \geq 0,$$

- and given **order-**$(n+1)$ method

$$\widetilde{w}_{j+1} = \widetilde{w}_j + h\,\widetilde{\phi}\,(t_j, \widetilde{w}_j, h)\,, \quad \text{for} \quad j \geq 0.$$

- for each j, compute

$$\begin{aligned} w_{j+1} &= w_j + h\,\phi\,(t_j, w_j, h)\,, \\ \widetilde{w}_{j+1} &= w_j + h\,\widetilde{\phi}\,(t_j, w_j, h)\,, \end{aligned}$$

- new step-size $q\,h$ should satisfy

$$q\,h \lesssim \left|\frac{\epsilon\,h}{\widetilde{w}_{j+1} - w_{j+1}}\right|^{\frac{1}{n}} h = \left|\frac{\epsilon}{\widetilde{\phi}\,(t_j, w_j, h) - \phi\,(t_j, w_j, h)}\right|^{\frac{1}{n}} h.$$

Runge-Kutta-Fehlberg: 4^{th} order method, 5^{th} order estimate

$$\begin{aligned} w_{j+1} &= w_j + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5, \\ \widetilde{w}_{j+1} &= w_j + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6, \quad \text{where} \end{aligned}$$

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$$
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k_1 &= h\,f\left(t_j, w_j\right), \\
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k_3 &= h\,f\left(t_j + \frac{3h}{8}, w_j + \frac{3}{32}\,k_1 + \frac{9}{32}\,k_2\right), \\
k_4 &= h\,f\left(t_j + \frac{12h}{13}, w_j + \frac{1932}{2197}\,k_1 - \frac{7200}{2197}\,k_2 + \frac{7296}{2197}\,k_3\right), \\
k_5 &= h\,f\left(t_j + h, w_j + \frac{439}{216}\,k_1 - 8\,k_2 + \frac{3680}{513}\,k_3 - \frac{845}{4104}\,k_4\right), \\
k_6 &= h\,f\left(t_j + \frac{h}{2}, w_j - \frac{8}{27}\,k_1 + 2\,k_2 - \frac{3544}{2565}\,k_3 + \frac{1859}{4104}\,k_4 - \frac{11}{40}\,k_5\right).
\end{aligned}
$$

Runge-Kutta-Fehlberg: step-size selection procedure

- compute a conservative value for q:

$$q = \left| \frac{\epsilon\, h}{\mathbf{2}\left(\widetilde{w}_{j+1} - w_{j+1}\right)} \right|^{\frac{1}{4}}.$$

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$$h = \begin{cases} 0.1\, h, & \text{if } q \leq 0.1, \\ 4\, h, & \text{if } q \geq 4. \end{cases}$$

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- step-size can't be too small:

$$\textbf{if} \quad h < h_{\mathbf{min}} \quad \textbf{then} \quad \textit{declare failure.}$$

Runge-Kutta-Fehlberg: example

Initial Value ODE $\quad \dfrac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$

exact solution $\quad y(t) = (1 + t)^2 - 0.5\, e^t.$

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t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

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t_j	h_j	$y(t_j)$	w_j	$\widetilde{w}_j$
0.00000	0.00000	0.50000	0.50000	0.50000
0.25000	0.25000	0.92049	0.92049	0.92049
0.48655	0.23655	1.39649	1.39649	1.39649
0.72933	0.24278	1.95374	1.95375	1.95375
0.97933	0.25000	2.58642	2.58643	2.58643
1.22933	0.25000	3.26045	3.26046	3.26046
1.47933	0.25000	3.95208	3.95210	3.95210
1.72933	0.25000	4.63081	4.63083	4.63083
1.97933	0.25000	5.25747	5.25749	5.25749
2.00000	0.02067	5.30547	5.30549	5.30549

Runge-Kutta-Fehlberg: solution plots

Initial Value ODE $$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Runge-Kutta-Fehlberg: solution plots

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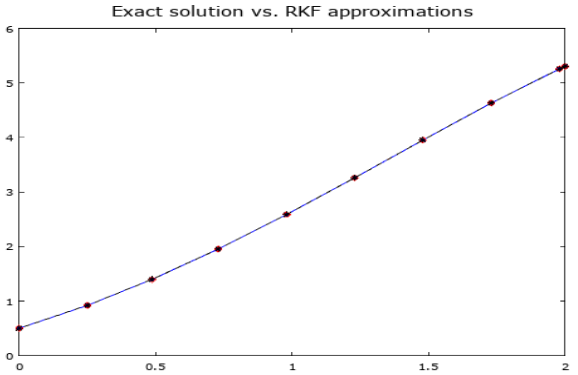

Runge-Kutta-Fehlberg: solution errors

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Runge-Kutta-Fehlberg: solution errors

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Runge-Kutta-Fehlberg: truncation errors

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$$\textbf{actual} \stackrel{def}{=} \left| \frac{y(t_j) - w_j}{h_j} \right|, \quad \textbf{estimate} \stackrel{def}{=} \left| \frac{\widetilde{w}_j - w_j}{h_j} \right|.$$

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