5.3.1 Modified Euler Method

Numerical solution of Initial Value Problem:

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = f(t,Y) \Leftrightarrow Y(t_{n+1}) = Y(t_n) + \int_{t_n}^{t_{n+1}} f(t,Y(t)) \, \mathrm{d}t.$$

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Approximate integral using the trapezium rule:

$$Y(t_{n+1}) \approx Y(t_n) + \frac{h}{2} [f(t_n, Y(t_n)) + f(t_{n+1}, Y(t_{n+1}))], \quad t_{n+1} = t_n + h.$$

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$$Y(t_{n+1}) \approx Y(t_n) + \frac{h}{2} [f(t_n, Y(t_n)) + f(t_{n+1}, \frac{Y(t_{n+1})}{(t_{n+1})})], \quad t_{n+1} = t_n + h.$$

Use Euler's method to approximate $Y(t_{n+1}) \approx Y(t_n) + hf(t_n, Y(t_n))$ in trapezium rule:

$$Y(t_{n+1}) \approx Y(t_n) + \frac{h}{2} [f(t_n, Y(t_n)) + f(t_{n+1}, Y(t_n) + hf(t_n, Y(t_n)))].$$

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Use Euler's method to approximate $Y(t_{n+1}) \approx Y(t_n) + hf(t_n, Y(t_n))$ in trapezium rule:

$$Y(t_{n+1}) \approx Y(t_n) + \frac{h}{2} \left[f(t_n, Y(t_n)) + f(t_{n+1}, Y(t_n) + hf(t_n, Y(t_n))) \right].$$

Hence the modified Euler's scheme

$$y_{n+1} = y_n + \frac{h}{2} \left[f(t_n, y_n) + f(t_{n+1}, y_n + hf(t_n, y_n)) \right] \Leftrightarrow \begin{cases} K_1 = hf(t_n, y_n) \\ K_2 = hf(t_{n+1}, y_n + K_1) \\ y_{n+1} = y_n + \frac{K_1 + K_2}{2} \end{cases}$$

Local truncation error due to the approximation:

$$Y(t_{n+1}) \approx Y(t_n) + \frac{1}{2}(K_1 + K_2)$$

where
$$K_1 = hf(t_n, Y(t_n))$$
 and $K_2 = hf(t_n + h, Y(t_n) + K_1)$.

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Taylor Series of $f(t_n + h, Y(t_n) + K_1)$ in two variables:

$$K_2 = h \left[f(t_n, Y(t_n)) + h \frac{\partial}{\partial t} f(t_n, Y(t_n)) + K_1 \frac{\partial}{\partial Y} f(t_n, Y(t_n)) + O\left(h^2, K_1^2\right) \right].$$

Local truncation error due to the approximation:

$$Y(t_{n+1})\approx Y(t_n)+\frac{1}{2}\left(K_1+K_2\right)$$

where $K_1 = hf(t_n, Y(t_n))$ and $K_2 = hf(t_n + h, Y(t_n) + K_1)$.

Taylor Series of $f(t_n + h, Y(t_n) + K_1)$ in two variables:

$$\label{eq:K2} \textit{K}_2 = \textit{h}\left[\textit{f}(\textit{t}_\textit{n}, \textit{Y}(\textit{t}_\textit{n})) + \textit{h}\frac{\partial}{\partial \textit{t}}\textit{f}(\textit{t}_\textit{n}, \textit{Y}(\textit{t}_\textit{n})) + \textit{K}_1\frac{\partial}{\partial \textit{Y}}\textit{f}(\textit{t}_\textit{n}, \textit{Y}(\textit{t}_\textit{n})) + \textit{O}\left(\textit{h}^2, \textit{K}_1^2\right)\right].$$

Since $K_1 = hf(t_n, Y(t_n)) = O(h)$,

$$\begin{split} \frac{1}{2} \left(\mathcal{K}_1 + \mathcal{K}_2 \right) &= h f(t_n, Y(t_n)) \\ &+ \frac{h^2}{2} \left[\frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O\left(h^3\right), \end{split}$$

Expression to be compared with Taylor expansion of $Y(t_{n+1})$

Taylor Series of
$$Y(t_{n+1}) = Y(t_n + h)$$
:

$$Y(t_n + h) = Y(t_n) + hY'(t_n) + \frac{h^2}{2}Y''(t_n) + O(h^3).$$

Taylor Series of $Y(t_{n+1}) = Y(t_n + h)$:

$$Y(t_n + h) = Y(t_n) + h \frac{Y'(t_n)}{2} + \frac{h^2}{2} Y''(t_n) + O(h^3).$$

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Substitute $Y'(t_n) = f(t_n, Y(t_n))$ and

$$\begin{aligned} Y''(t_n) &= \frac{\mathrm{d}}{\mathrm{d}t} f(t, Y(t)) \bigg|_{t_n} = \frac{\partial}{\partial t} f(t_n, Y(t_n)) + \frac{\mathrm{d}}{\mathrm{d}t} Y(t_n) \frac{\partial}{\partial Y} f(t_n, Y(t_n)), \\ &= \frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)), \end{aligned}$$

Taylor Series of $Y(t_{n+1}) = Y(t_n + h)$:

$$Y(t_n + h) = Y(t_n) + hY'(t_n) + \frac{h^2}{2}Y''(t_n) + O(h^3).$$

Substitute $Y'(t_n) = f(t_n, Y(t_n))$ and

$$Y''(t_n) = \frac{\mathrm{d}}{\mathrm{d}t} f(t, Y(t)) \bigg|_{t_n} = \frac{\partial}{\partial t} f(t_n, Y(t_n)) + \frac{\mathrm{d}}{\mathrm{d}t} Y(t_n) \frac{\partial}{\partial Y} f(t_n, Y(t_n)),$$

$$= \frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)),$$

to get

$$Y(t_n + h) = Y(t_n) + hf(t_n, Y(t_n))$$

$$+ \frac{h^2}{2} \left[\frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O\left(h^3\right). \quad (5.10)$$

Now, the equations

$$Y(t_{n+1}) = Y(t_n) + hf(t_n, Y(t_n))$$

$$+ \frac{h^2}{2} \left[\frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O\left(h^3\right)$$

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and

$$\begin{split} \frac{1}{2}\left(K_{1}+K_{2}\right) &= hf(t_{n},Y(t_{n})) \\ &+ \frac{h^{2}}{2}\left[\frac{\partial}{\partial t}f(t_{n},Y(t_{n})) + f(t_{n},Y(t_{n}))\frac{\partial}{\partial Y}f(t_{n},Y(t_{n}))\right] + O\left(h^{3}\right) \end{split}$$

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imply that
$$Y(t_{n+1}) = Y(t_n) + \frac{1}{2}(K_1 + K_2) + \frac{O(h^3)}{h^3}$$
.

The local truncation error is $\tau_n = O\left(h^3\right)$: the modified Euler method is second order accurate. (A method is conventionally called p^{th} order if the local truncation error is of order p+1.)

5.3.2 Second order Runge-Kutta schemes (1/3)

Modified Euler is an example of $2^{\rm nd}$ order R-K method.

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The general 2nd order Runge-Kutta scheme takes the form

$$\begin{cases}
K_1 = hf(t_n, y_n); \\
K_2 = hf(t_n + \alpha h, y_n + \beta K_1); \\
y_{n+1} = y_n + a_1 K_1 + a_2 K_2.
\end{cases} (5.11)$$

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\end{cases} (5.11)$$

Repeating the earlier analysis, $K_1 = hf(t_n, Y(t_n))$ and

$$egin{aligned} \mathcal{K}_2 &= hf(t_n, Y(t_n)) \ &+ h^2 \left[lpha rac{\partial}{\partial t} f(t_n, Y(t_n)) + eta f(t_n, Y(t_n)) rac{\partial}{\partial Y} f(t_n, Y(t_n))
ight] + O(h^3); \end{aligned}$$

$$\Rightarrow a_1K_1 + a_2K_2 = h(a_1 + a_2)f(t_n, Y(t_n)) + a_2h^2 \left[\alpha \frac{\partial}{\partial t} f(t_n, Y(t_n)) + \beta f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O(h^3).$$

5.3.2 Second order Runge-Kutta schemes (2/3)

Comparing

$$\begin{aligned} a_1K_1 + a_2K_2 &= h(a_1 + a_2)f(t_n, Y(t_n)) \\ &+ a_2h^2\left[\alpha\frac{\partial}{\partial t}f(t_n, Y(t_n)) + \beta f(t_n, Y(t_n))\frac{\partial}{\partial Y}f(t_n, Y(t_n))\right] + O(h^3) \end{aligned}$$

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with equation (5.10)

$$Y(t_{n+1}) = Y(t_n) + hf(t_n, Y(t_n))$$

$$+ \frac{h^2}{2} \left[\frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O(h^3),$$

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$$\begin{aligned} a_1K_1 + a_2K_2 &= h(a_1 + a_2)f(t_n, Y(t_n)) \\ &+ a_2h^2\left[\alpha\frac{\partial}{\partial t}f(t_n, Y(t_n)) + \beta f(t_n, Y(t_n))\frac{\partial}{\partial Y}f(t_n, Y(t_n))\right] + O(h^3) \end{aligned}$$

with equation (5.10)

$$\begin{split} Y(t_{n+1}) &= Y(t_n) + hf(t_n, Y(t_n)) \\ &+ \frac{h^2}{2} \left[\frac{\partial}{\partial t} f(t_n, Y(t_n)) + f(t_n, Y(t_n)) \frac{\partial}{\partial Y} f(t_n, Y(t_n)) \right] + O\left(h^3\right), \end{split}$$

one gets a second order scheme $Y(t_{n+1}) = Y(t_n) + a_1K_1 + a_2K_2 + O\left(h^3\right)$ if

$$\begin{cases} a_1 + a_2 = 1; \\ \alpha a_2 = \beta a_2 = \frac{1}{2}. \end{cases}$$
 (5.12)

5.3.2 Second order Runge-Kutta Schemes (3/3)

General 2nd order Runge-Kutta scheme:

$$\begin{cases} K_1 = hf(t_n, y_n); \\ K_2 = hf(t_n + \alpha h, y_n + \beta K_1); \\ y_{n+1} = y_n + a_1 K_1 + a_2 K_2. \end{cases} \text{ with } \begin{cases} a_1 + a_2 = 1; \\ \alpha a_2 = \beta a_2 = \frac{1}{2}. \end{cases}$$

Since we have 3 equations and 4 unknowns $(a_1, a_2, \alpha, \beta)$, there are infinitely many solutions.

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$$\begin{cases} K_1 = hf(t_n, y_n); \\ K_2 = hf(t_n + \alpha h, y_n + \beta K_1); \\ y_{n+1} = y_n + a_1 K_1 + a_2 K_2. \end{cases} \text{ with } \begin{cases} a_1 + a_2 = 1; \\ \alpha a_2 = \beta a_2 = \frac{1}{2}. \end{cases}$$

Since we have 3 equations and 4 unknowns $(a_1, a_2, \alpha, \beta)$, there are infinitely many solutions.

The most popular are,

- ▶ Modified Euler: $a_1 = a_2 = 1/2$, $\alpha = \beta = 1$. ⇒ $K_1 = hf(t_n, y_n)$, $K_2 = hf(t_n + h, y_n + K_1)$ and $y_{n+1} = y_n + (K_1 + K_2)/2$.
- ▶ Midpoint method: $a_1 = 0$, $a_2 = 1$, $\alpha = \beta = 1/2$. ⇒ $K_1 = hf(t_n, y_n)$, $K_2 = hf(t_n + h/2, y_n + K_1/2)$ and $y_{n+1} = y_n + K_2$.
- ▶ Heun's method: $a_1 = 1/4$, $a_2 = 3/4$, $\alpha = \beta = 2/3$. ⇒ $K_1 = hf(t_n, y_n)$, $K_2 = hf(t_n + 2h/3, y_n + 2K_1/3)$ and $y_{n+1} = y_n + (K_1 + 3K_2)/4$.

5.3.3 Higher order Runge-Kutta methods

Schemes of the form (5.11) can be extended to higher order methods. The most widely used Runge-Kutta scheme is the 4^{th} order scheme RK4 based on Simpson's rule.

$$y_{n+1} = y_n + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4),$$
where $K_1 = hf(t_n, y_n),$

$$K_2 = hf\left(t_n + \frac{h}{2}, y_n + \frac{K_1}{2}\right),$$

$$K_3 = hf\left(t_n + \frac{h}{2}, y_n + \frac{K_2}{2}\right),$$

$$K_4 = hf(t_n + h, y_n + K_3).$$
(5.13)

This scheme has local truncation error of order h^5 , which can be checked in the same way as the second order scheme, but involves rather messy algebra.