Initial Value Problem

$$\begin{cases} y'(t) = f(t, y(t)), & t > a, \\ y(a) = y_a. \end{cases}$$

Numerical approximation

$$\begin{aligned} a &= t_0 < t_1 < \cdots < t_N = b, \\ h &= t_{i+1} - t_i, \\ w_i &\approx y(t_i), \end{aligned}$$

E.g.: forward Euler

$$w_{i+1} = w_i + hf(t_i, w_i)$$

One-step vs global errors

One-step error

Error commited after one step of the method.

- Assume: $w_{i-1} = y(t_{i-1})$
- After one step: $e_i = |w_i - y(t_i)|$
- Computation/estimation: Taylor series expansion.

Example: forward Euler

$$\begin{aligned} y(t_{i+1}) = y(t_i + h) &= y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\tau) \\ &= \underbrace{y(t_i) + hf(t_i, y(t_i))}_{\text{frw. Euler}} + \frac{h^2}{2}y''(\tau), \end{aligned}$$

$$e_{i+1} = \frac{h^2}{2}|y''(\tau)| = O(h^2)$$

One-step vs global errors

Global error

Difference btw. analytical and numerical solution (error after many steps of the method).

- Assume: $w_0 = y(t_0)$
- Global error: $g_i = |w_i - y(t_i)|$.
- Estimate:
  - f-uniformly Lipschitz in y with constant L
  - all solutions exist and unique etc
  - one-step error $e_i \leq Ch^{k+1}$

$$g_i \leq \frac{Ch^k}{L}(e^{L(t_i - a)} - 1)$$

Lessons learned:

Small one-step error + small Lipschitz constant of f + smooth $y(t)$ (use Taylor expansions) $\implies$ small global error!

Derivation: central differences

Taylor series expansion around $t_i + \frac{h}{2}$:

$$y(t_i + h) = y(t_i + \tfrac{h}{2}) + y'(t_i + \tfrac{h}{2})\tfrac{h}{2} + y''(t_i + \tfrac{h}{2})\frac{(\frac{h}{2})^2}{2} + y'''(\tau_1)\frac{(\frac{h}{2})^3}{3!},$$

$$y(t_i) = y(t_i + \tfrac{h}{2}) - y'(t_i + \tfrac{h}{2})\tfrac{h}{2} + y''(t_i + \tfrac{h}{2})\frac{(\frac{h}{2})^2}{2} - y'''(\tau_2)\frac{(\frac{h}{2})^3}{3!},$$

Subtract the two:

$$y(t_i + h) - y(t_i) = hy'(t_i + \tfrac{h}{2}) + h^3\frac{y'''(\tau_3)}{24}$$

Contrast with forward Euler:

$$y(t_i + h) - y(t_i) = hy'(t_i) + h^2\frac{y''(\tau)}{2}$$

Derivation: central differences

Taylor series expansion around $t_i + \frac{h}{2}$:

$$y(t_i + h) = y(t_i + \tfrac{h}{2}) + y'(t_i + \tfrac{h}{2})\tfrac{h}{2} + y''(t_i + \tfrac{h}{2})\frac{(\frac{h}{2})^2}{2} + y'''(\tau_1)\frac{(\frac{h}{2})^3}{3!},$$

$$y(t_i) = y(t_i + \tfrac{h}{2}) - y'(t_i + \tfrac{h}{2})\tfrac{h}{2} + y''(t_i + \tfrac{h}{2})\frac{(\frac{h}{2})^2}{2} - y'''(\tau_2)\frac{(\frac{h}{2})^3}{3!},$$

Subtract the two:

$$y(t_i + h) - y(t_i) = hy'(t_i + \tfrac{h}{2}) + h^3\frac{y'''(\tau_3)}{24}$$

Add the two:

$$\frac{y(t_i + h) + y(t_i)}{2} = y(t + \tfrac{h}{2}) + h^2 y''(t_i + \tfrac{h}{2}) + \text{smaller terms}$$

Explicit Runge–Kutta methods

$$
\begin{aligned}
w_{n+1} &= w_n + h \sum_{i=1}^{s} b_i k_i, \\
k_1 &= f(t_n, w_n), \\
k_2 &= f(t_n + c_2 h, w_n + h(a_{21} k_1)), \\
k_3 &= f(t_n + c_3 h, w_n + h(a_{31} k_1 + a_{32} k_2)), \\
&\vdots \\
k_s &= f(t_n + c_s h, w_n + h(a_{s1} k_1 + a_{s2} k_2 + \cdots + a_{s,s-1} k_{s-1}))
\end{aligned}
$$

- s: no. of stages
- c_i: nodes
- b_i: weights
- a_{ij}: Runge–Kutta matrix

Butcher tableau

$$
\begin{array}{c|ccccc}
0 & & & & \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & a_{32} & & \\
\vdots & \vdots & & \ddots & \\
c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1}
\end{array}
$$

Forward Euler

$$w_{n+1} = w_n + hf(t, w_n)$$

$$
\begin{array}{c|c}
0 & \\
\hline
 & 1
\end{array}
$$

Midtpoint

$$
\begin{aligned}
w_{n+1} &= w_n + hk_2 \\
k_1 &= f(t_n, w_n), \\
k_2 &= f(t_n + h/2, w_n + h/2k_1),
\end{aligned}
$$

$$
\begin{array}{c|cc}
0 & & \\
1/2 & 1/2 & \\
\hline
 & 0 & 1
\end{array}
$$

Explicit trapezoid

$$
\begin{aligned}
w_{n+1} &= w_n + h/2(k_1 + k_2) \\
k_1 &= f(t_n, w_n), \\
k_2 &= f(t_n + h, w_n + hk_1),
\end{aligned}
$$

$$
\begin{array}{c|cc}
0 & & \\
1 & 1 & \\
\hline
 & 1/2 & 1/2
\end{array}
$$

RK4 “The Runge–Kutta method”

$$
\begin{array}{c|cccc}
0 & & & & \\
1/2 & 1/2 & & & \\
1/2 & 0 & 1/2 & & \\
1 & 0 & 0 & 1 & \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$

- 4 stages
- One step error: $O(h^5)$
- Global error: $O(h^4)$

Implicit (Runge-Kutta) methods

(Implicit)Trapezoid method

$$w_{n+1} = w_n + h/2(f(t_n, w_n) + f(t_n + h, w_{n+1}))$$

Implicit/backward Euler method

$$w_{n+1} = w_n + hf(t_n + h, w_{n+1})$$

Implicit Runge–Kutta methods

$$w_{n+1} = w_n + h \sum_{i=1}^{s} b_i k_i,$$

$$k_1 = f\left(t_n + c_1 h, w_n + \sum_{i=1}^{s} a_{1i} k_i\right),$$

$$k_2 = f\left(t_n + c_2 h, w_n + \sum_{i=1}^{s} a_{2i} k_i\right),$$

$$\vdots$$

$$k_s = f\left(t_n + c_s h, w_n + \sum_{i=1}^{s} a_{si} k_i\right),$$

- s: no. of stages
- c_i: nodes
- b_i: weights
- a_{ij}: Runge–Kutta matrix

Butcher tableau: Implicit Euler

$$w_{n+1} = w_n + hf(t_n + h, w_{n+1}),$$

or

$$\begin{aligned} w_{n+1} &= w_n + hk_1, \\ k_1 &= f(t_n + h, w_n + hk_1), \end{aligned}$$

Butcher tableau:

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$

Butcher tableau: Trapezoid method

$$w_{n+1} = w_n + h/2(f(t_n, w_n) + f(t_n + h, w_{n+1})),$$

or

$$\begin{aligned} w_{n+1} &= w_n + h/2(k_1 + k_2), \\ k_1 &= f(t_n, w_n), \\ k_2 &= f(t_n + h, w_n + h/2(k_1 + k_2)) \end{aligned}$$

Butcher tableau:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$