Ordinary differential equations

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Initial Value Problem

$$\begin{cases} y'(t) = f(t, y), & t \geq t_0 \\ y(t_0) = y_0 \end{cases}$$

- $y : \mathbb{R} \to \mathbb{R}^n$ is searched
- $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is given
- $t_0 \geq 0$ and $y_0 \in \mathbb{R}^n$ are given
- $y' = \frac{\mathrm{d}y}{\mathrm{d}t}$ denotes derivative with respect to t:

$$y' = \begin{bmatrix} y_1'(t) \\ y_2'(t) \\ \dots \\ y_n'(t) \end{bmatrix} = \begin{bmatrix} \mathrm{d}y_1(t)/\mathrm{d}t \\ \mathrm{d}y_2(t)/\mathrm{d}t \\ \dots \\ \mathrm{d}y_n(t)/\mathrm{d}t \end{bmatrix}$$

Autonomous Initial Value Problem

Autonomous Initial Value Problem is of the form:

$$\begin{cases} y'(t) = f(y) \\ y(t_0) = y_0 \end{cases}$$

Every Initial Value Problem

$$\begin{cases} y'(t) = f(t, y) \\ y(t_0) = y_0 \end{cases}$$

can be transformed to autonomous Initial Value Problem by introducing a new variable $y_{n+1}(t) = t$

$$\begin{bmatrix} y(t) \\ y_{n+1}(t) \end{bmatrix}' = \begin{bmatrix} f(y_{n+1}, y) \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} y(t_0) \\ y_{n+1}(t_0) \end{bmatrix} = \begin{bmatrix} y_0 \\ t_0 \end{bmatrix}$$

Local existence and uniqueness

Theorem (Local existence)

If $f(t,y)$ is continuous in a rectangle centered around (t_0, y_0):
$D = \{ (t,y) \mid |t - t_0| \leq \alpha, |y - y_0| \leq \beta \}$
then the IVP has a solution $y(t)$ for $|t - t_0| \leq \min(\alpha, \beta/M)$, where $M = \max_{(t,y)\in D} |f(t,y)|$.

Theorem (Local existence and uniqueness)

If $f(t,y)$ and $\frac{\partial}{\partial y} f(t,y)$ are continuous in a rectangle centered around (t_0, y_0): $D = \{ (t,y) \mid |t - t_0| \leq \alpha, |y - y_0| \leq \beta \}$
then the IVP has a unique solution $y(t)$ for
$|t - t_0| \leq \min(\alpha, \beta/M)$, *where* $M = \max_{(t,y)\in D} |f(t,y)|$.

Lipschitz continuity

Lipschitz continuity.

Function $f(t,y)\colon \mathbb{R}^{n+1} \to \mathbb{R}^n$ is Lipschitz continuous if there is constant L (independent of time) such, that for any $t \in [a,b]$ and any $y_2, y_1 \in \Omega$

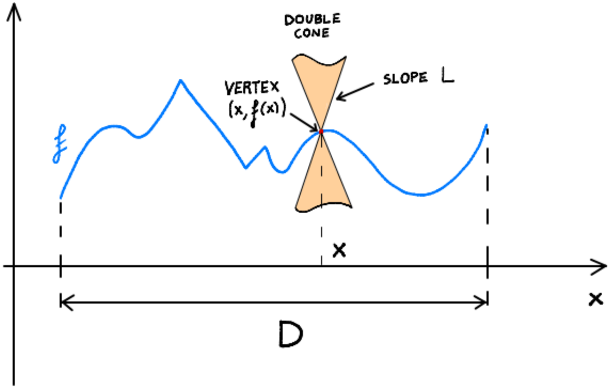
$$||f(t,y_2) - f(t,y_1)|| \leq L||y_2 - y_1||$$

Remark. If f is differentiable:

$$L = \max_{(t,y)\in D} ||J_f(t,y)||$$

Example.
$y = x^2$ is Lipschitz continuous on $[0, x_0]$ but is not Lipschitz continuous on $\mathbb{R}$.

Lipschitz continuity



Global existence and uniqueness

Picard-Lindelöf theorem

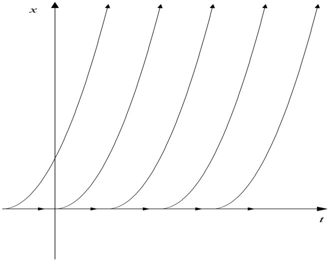
Theorem (Global existence and uniqueness)

If $f(t, y)$ is continuous in a strip $a \leq t \leq b, \ -\infty \leq y \leq \infty$ and uniformly Lipschitz continuous in y
then the IVP has a unique solution $y(t)$ for $t \in [a, b]$.

Existence and Uniqueness

$$\begin{cases} y' = y^{1/2}, \; y \geq 0 \\ y(0) = 0 \end{cases}$$

$$y(t) = \begin{cases} 0, & \text{for } 0 \leq t \leq C \\ \frac{1}{4}(t - C)^2, & \text{for } C \leq t \leq \infty \end{cases}$$



- Lack of uniqueness
- Infinite family of solutions exists
- Function $f(t, y) = y^{1/2}$ is not Lipschitz continuous near $y = 0$

Existence and Uniqueness

$$\begin{cases} y' = y^{1/3} \\ y(0) = 0 \end{cases}$$

Solutions:

$$y(t) \equiv 0$$

$$y(t) = \begin{cases} 0, & \text{for } 0 \le t \le C \\ \left(\frac{2}{3}(t-C)\right)^{3/2}, & \text{for } C \le t \le \infty \end{cases}$$

$$y(t) = \begin{cases} 0, & \text{for } 0 \le t \le C \\ -\left(\frac{2}{3}(t-C)\right)^{3/2}, & \text{for } C \le t \le \infty \end{cases}$$

Two infinite families of solutions exist

Local existence

$$\begin{cases} y' = y^2 \\ y(0) = 1 \end{cases}$$

Solution $y(t) = \frac{1}{1-t}$ is valid only for $t \in (-\infty, 1)$.

- Lack of global solution
- Only local solution exists
- Solution $y(t) = \frac{1}{1-t}$ blows-up at $t = 1$
- Function $f(t, y) = y^2$ is not globally Lipschitz continuous

Local existence

$$\begin{cases} y' = y\tan(t) \\ y(0) = 1 \end{cases}$$

Solution $y(t) = \frac{1}{\cos(t)}$ is valid only for $-\frac{\pi}{2} < t < \frac{\pi}{2}$.

- Lack of global solution
- Only local solution exists
- Solution $y(t) = \frac{1}{\cos(t)}$ blows-up at $t = \pm\frac{\pi}{2}$
- Function $f(t, y) = y\tan(t)$ is not Lipschitz continuous near $\pm\frac{\pi}{2}$ w.r.t y

Let us suppose that $f(t, y)$ is Lipschitz continuous. Then
$|y_2\tan(t) - y_1\tan(t)| \leq L|y_2 - y_1|$
$|(y_2 - y_1)| \cdot |\tan(t)| \leq L|y_2 - y_1|$
$|\tan(t)| \leq L$
But L is a constant independent of t, while $|\tan(t)|$ can be arbitrarily large, which contradicts Lipschitz continuity of $f(t, y)$.

Local existence

$$\begin{cases} y' = -y^{-1/2} \\ y(0) = 1 \end{cases}$$

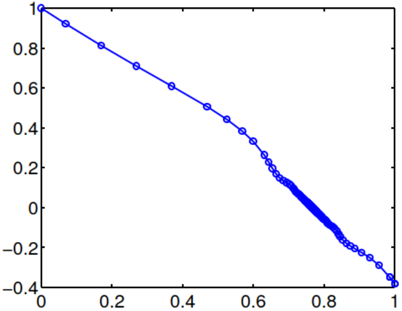
Solution $y(t) = (1 - \frac{3}{2}t)^{2/3}$ is valid only for $t < \frac{2}{3}$.

- Lack of global solution
- Only local solution exists
- For $t = \frac{2}{3}$ we would have $y(t) = 0$ making $f(t, y) = -\frac{1}{\sqrt{y}}$ undefined

Local existence

$$\begin{cases} y' = \sin(1/y) - 2 \\ y(0) = 1 \end{cases}$$

Solution $y(t)$ is valid only for $t < 0.76741$.



- Lack of global solution
- Only local solution exists
- For $t \approx 0.76741$ we would have $y(t) = 0$ making $\sin(1/y)$ undefined
- Numerical solver does not see it

Local and global error

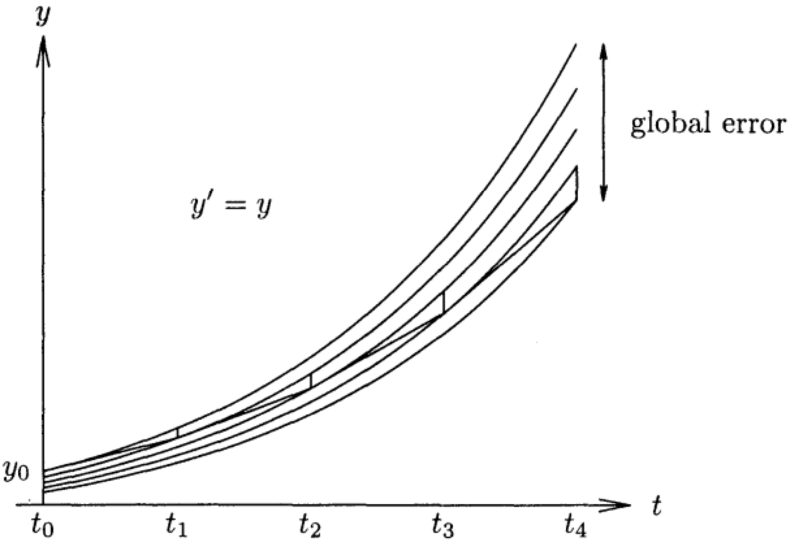
Local error [2]

$$\ell_k(h) = \frac{y_k - u_{k-1}(t_k)}{h_k} \tag{1}$$

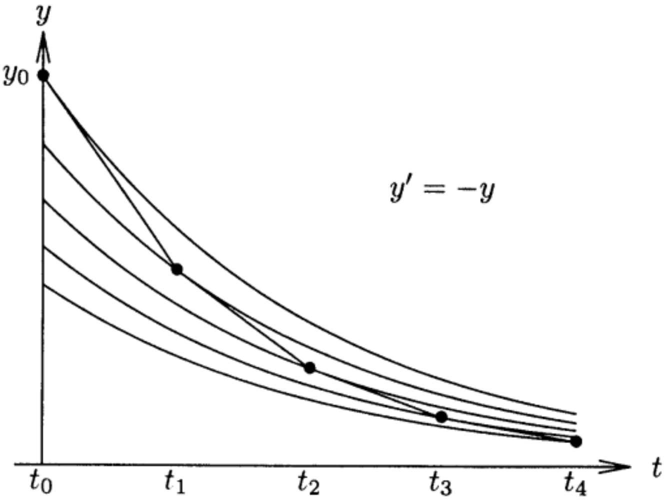
Global error

$$e_k(h) = y_k - y(t_k) \tag{2}$$

Local and global error



Local and global error



Properties of numerical solutions

Consistency	concerns local error
Convergence	concerns global error
Stability	concerns initial conditions

Properties of numerical solutions

A numerical scheme is consistent if for any n:

$$\lim_{h \to 0} \frac{\ell_n(h)}{h} \to 0 \tag{3}$$

For one-step solvers if the local error is $O(h^{p+1})$ then the global error is $O(h^p)$.

For one-step solvers:

$$\text{convergence} \Leftrightarrow \text{consistency}$$

For multistep-step solvers:

$$\text{convergence} \Leftrightarrow \text{consistency} + \text{zero stability}$$

Stability

- Convergence concerns situation when $h \to 0$.
- We are interested in situation when h is small, but not too small. Otherwise our method would be computationally inefficient.
- Behaviour in such situation is described by stability.

Stability of Initial Value Problem

$$\begin{cases} y' = f(y,t) \\ y(t_0) = y_0 \end{cases} \qquad \begin{cases} z' = f(z,t) \\ z(t_0) = z_0 \end{cases} \tag{4}$$

Solution to IVP (4) is stable if for every ε there exists δ such that if

$$||z(t_0) - y(t_0)|| < \delta$$

then

$$||z(t) - y(t)|| < \varepsilon \text{ for } t \geq t_0.$$

Stable solution to $y' = f(y,t)$ is asymptotically stable if

$$||z(t) - y(t)|| \to 0 \text{ for } t \to \infty.$$

Sense: IVP is well-conditioned or well-posed?

Dahlquist's test equation

Dahlquist's test equation

$$y' = \lambda y,\ \ t \geq 0,\ \ \lambda \in \mathbb{C} \tag{5}$$

Let us restrict to cases:

$$y' = \lambda y,\ \ t \geq 0,\ \ \lambda < 0 \tag{6}$$

Exact solution:

$$y(t) = y_0 e^{\lambda t} \tag{7}$$

Forward Euler method

Other name: Explicit Euler method

$$y_{n+1} = y_n + hf(t_n, y_n) \tag{8}$$

Numerical stability:

$$|1 + h\lambda| < 1 \tag{9}$$

$$0 < h < -\frac{2}{\lambda} \tag{10}$$

Backward Euler method

Other name: Implicit Euler method

$$y_{n+1} = y_n + hf(t_{n+1}, y_{n+1}) \tag{11}$$

Numerical stability:

$$\left| \frac{1}{1 - h\lambda} \right| < 1 \tag{12}$$

$$h > 0 \tag{13}$$

Trapezoidal method

Other names: Crank-Nicolson metod

$$y_{n+1} = y_n + \frac{h}{2}[f(t_n, y_n) + f(t_{n+1}, y_{n+1})] \tag{14}$$

Numerical stability:

$$\left| \frac{1 + \frac{1}{2}\lambda h}{1 - \frac{1}{2}\lambda h} \right| < 1 \tag{15}$$

$$h > 0 \tag{16}$$

Modified Euler

Second-order Runge-Kutta method
Other names: Improved Euler, Heun method
Predictor-corrector method:

- Predictor: Forward Euler method
- Corrector: Trapezoidal method

$$\tilde{y}_{n+1} = y_n + h_k f(t_n, y_n) \tag{17}$$

$$y_{n+1} = y_n + \frac{h}{2}[f(t_n, y_n) + f(t_{n+1}, \tilde{y}_{n+1})] \tag{18}$$

Numerical stability:

$$\left| 1 + \lambda h + \frac{1}{2}(\lambda h)^2 \right| < 1 \tag{19}$$

$$0 < h < -\frac{2}{\lambda} \tag{20}$$

Midpoint method

Second-order Runge-Kutta method

$$y_{n+1} = y_n + hf\left(t_{n+1/2}, y(t_{n+1/2})\right) \tag{21}$$

We do not know $y(t_{n+1/2}) \equiv y(t_n + h/2)$

- Replacing $y(t_{n+1/2})$ with $y_n + \frac{h}{2}f(t_n, y_n)$ we get explicit midpoint method
- Replacing $y(t_{n+1/2})$ with $\frac{y_n+y_{n+1}}{2}$ we get implicit midpoint method
- Taking step $2h$ instead of h in (21) we get leapfrog method

Midpoint method

Explicit midpoint method

$$y_{n+1} = y_n + hf\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} f(t_n, y_n)\right) \tag{22}$$

Implicit midpoint method

$$y_{n+1} = y_n + hf\left(t_n + \frac{h}{2}, \frac{y_n + y_{n+1}}{2}\right) \tag{23}$$

Leapfrog method

$$y_{n+1} = y_{n-1} + 2hf(t_n, y_n) \tag{24}$$

Runge-Kutta 4

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{25}$$

$$k_1 = f(t_n, y_n) \tag{26}$$

$$k_2 = f(t_n + h/2, y_n + hk_1/2) \tag{27}$$

$$k_3 = f(t_n + h/2, y_n + hk_2/2) \tag{28}$$

$$k_4 = f(t_n + h, y_n + hk_3) \tag{29}$$

Numerical stability:

$$\left|1 + \lambda h + \frac{1}{2}(\lambda h)^2 + \frac{1}{6}(\lambda h)^3 + \frac{1}{24}(\lambda h)^4\right| < 1 \tag{30}$$

$$0 < h < -\frac{2.8}{\lambda} \tag{31}$$

Runge-Kutta 3/8

$$y_{n+1} = y_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4) \tag{32}$$

$$k_1 = f(t_n, y_n) \tag{33}$$

$$k_2 = f(t_n + \frac{1}{3}h, y_n + \frac{1}{3}hk_1) \tag{34}$$

$$k_3 = f(t_n + \frac{2}{3}h, y_n - \frac{1}{3}hk_1 + hk_2) \tag{35}$$

$$k_4 = f(t_n + h, y_n + hk_1 - hk_2 + hk_3) \tag{36}$$

- Smaller error coefficients than in RK4
- Requires slightly more flops per time step than RK4

Runge-Kutta-Fehlberg

$$
\begin{aligned}
k_1 &= f(t_n, y_n) \\
k_2 &= f(t_n + \frac{1}{4}h, y_n + \frac{1}{4}hk_1) \\
k_3 &= f(t_n + \frac{3}{8}h, y_n + \frac{3}{32}hk_1 + \frac{9}{32}hk_2) \\
k_4 &= f(t_n + \frac{12}{13}h, y_n + \frac{1932}{2197}hk_1 - \frac{7200}{2197}hk_2 + \frac{7296}{2197}hk_3) \\
k_5 &= f(t_n + h, y_n + \frac{439}{216}hk_1 - 8hk_2 + \frac{3680}{513}hk_3 - \frac{845}{4104}hk_4) \\
k_6 &= f(t_n + \frac{1}{2}h, y_n - \frac{8}{27}hk_1 + 2hk_2 - \frac{3544}{2655}hk_3 + \frac{1859}{4104}hk_4 - \frac{11}{40}hk_5)
\end{aligned}
$$

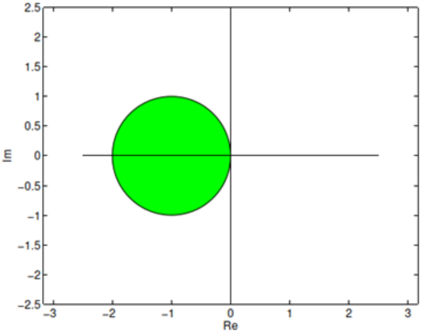
$$
\begin{aligned}
y_{n+1} &= y_n + h(\frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5) \\
\hat{y}_{n+1} &= y_n + h(\frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6)
\end{aligned}
$$

Amplification factor

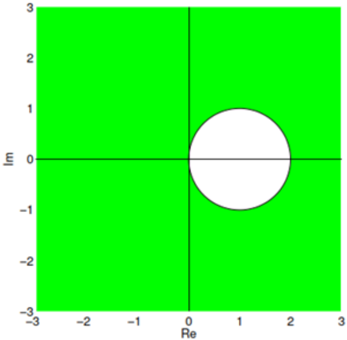
$$\varepsilon_{n+1} = Q(\lambda h)\varepsilon_n \tag{37}$$

Method	Amplification factor
Explicit Euler	$1 + \lambda h$
Implicit Euler	$\frac{1}{1-\lambda h}$
Trapezoidal	$\frac{1+\frac{1}{2}\lambda h}{1-\frac{1}{2}\lambda h}$
Modified Euler	$1 + \lambda h + \frac{1}{2}(\lambda h)^2$
RK4	$1 + \lambda h + \frac{1}{2}(\lambda h)^2 + \frac{1}{6}(\lambda h)^3 + \frac{1}{24}(\lambda h)^4$

Stability regions

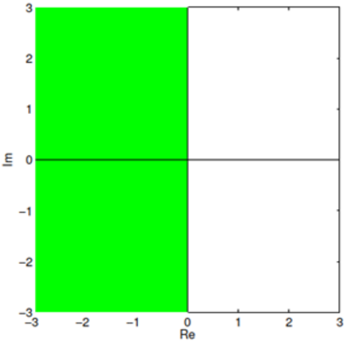


(a) Explicit Euler method

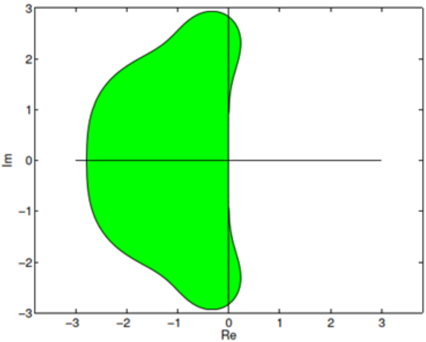


(b) Implicit Euler method

Stability regions



(c) Implicit trapezoidal rule



(d) Explicit Runge-Kutta method (RK4)

Linear system of ODEs

$$y' = Ay \tag{38}$$

Euler method is stable if for each eigenvalue λ of A:

$$|1 + \lambda h| < 1 \tag{39}$$

$$0 < h < \frac{2}{\max\{|\lambda| \mid \lambda \text{ is eigenvalue of } A\}} \tag{40}$$

Local error

Method	Local error	Global error	Order
Explicit Euler	$O(h)$	$O(h)$	1
Implicit Euler	$O(h)$	$O(h)$	1
Trapezoidal	$O(h^2)$	$O(h^2)$	2
Modified Euler	$O(h^2)$	$O(h^2)$	2
Midpoint method	$O(h^2)$	$O(h^2)$	2
Leapfrog method	$O(h^2)$	$O(h^2)$	2
RK4	$O(h^4)$	$O(h^4)$	4

Step size

Limitations on maximum step size h have three sources:

- Accuracy of numerical solution
- Stability of numerical solution
- Convergence of generally nonlinear equation $y_{n+1} = \underbrace{y_n + h\Psi(y_{n+1})}_{\phi(y_{n+1})}$ solved when using implicit methods
- If limitations on step size due to stablity are more severe than due to desired accuracy we say that solved ODE is stiff
- Limitations on step size may also arise when solving nonlinear equation for implicit method with direct iteration $y_{n+1} = \phi(y_{n+1})$. In such cases Newton method should be used, which is however more costly.

Methods

Fixed step	Adaptive step
Euler method	Runge-Kutta 1(2), Adaptive Heun
Midpoint method	Runge-Kutta 2(3), Bogacki-Shampine
Runge-Kutta 4, 3/8 rule	Runge-Kutta 4(5), Dormand-Prince
Explicit Adams-Bashforth	Runge-Kutta 7(8), Dormand-Prince-Shampine
Implicit Adams-Bashforth-Moulton	

Conservation laws

Method	Symplectic	Energy	Angular momentum
Explicit Euler	$\times$	$\nearrow$	$\times$
Implicit Euler	$\times$	$\searrow$	$\times$
Semi explicit Euler	$\checkmark$	$\times$	$\checkmark$
RK4	$\times$		

References

[1] Michael T. Heath,
http://heath.cs.illinois.edu/scicomp/notes/cs450_chapt09.pdf

[2] C. Vuik, F.J. Vermolen, M.B. van Gijzen, M.J. Vuik,
Numerical Methods for Ordinary Differential Equations