Ordinary Differential Equations

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Problem Formulation

We are interested in computing the solution $x : [t_0, t_1] \to \mathbb{R}^n$ of the ordinary differential equations (ODE)

$$\forall\, t \in [t_0, t_1], \quad \dot{x}(t) = f(x(t)) \text{ with } x(t_0) = x_0.$$

Assumptions:

- The function $f : \mathbb{R}^n \to \mathbb{R}^n$ is smooth.
- The initial value $x_0 \in \mathbb{R}^n$ is given.

Explicit Time Dependence

- **Important:** In practice, ODEs are often explicit time-dependet

$$\forall\, t \in [t_0, t_1], \quad \dot{y}(t) = g(t, y(t)) \;\text{ with }\; y(t_0) = y_0.$$

- **But** for theoretical derivations we may define

$$x(t) = \begin{bmatrix} y(t) \\ t \end{bmatrix},\; f(x) = \begin{bmatrix} g(t, y(t)) \\ 1 \end{bmatrix},\; \text{and} \;\; x_0 = \begin{bmatrix} y(t_0) \\ t_0 \end{bmatrix}.$$

Integral Form

The ordinary differential equation (ODE)

$$\forall\, t \in [t_0, t_1], \quad \dot{x}(t) = f(x(t)) \text{ with } x(t_0) = x_0$$

can be equivalently be written in its integral form

$$\forall\, t \in [t_0, t_1], \quad x(t) = x_0 + \int_{t_0}^{t} f(x(\tau))\mathrm{d}\tau.$$

Lipschitz Continuity

Definition:

- The function f is called (globally) Lipschitz continuous, if there exist a constant $L < \infty$ with

$$\forall\, x, y \in \mathbb{R}^n, \quad \|f(x) - f(y)\| \leq L \, \|x - y\| \, .$$

Existence and Uniqueness

Theorem (Picard-Lindelöf):

- If f is globally Lipschitz continuous, the ODE has a unique solution.

Sketch proof:

1. Start with any continuous function $y_1 : [t_0, t_1] \to \mathbb{R}^n$ and iterate

$$y_{i+1}(t) = x_0 + \int_{t_0}^{t} f(y_i(\tau))\mathrm{d}\tau \qquad \text{[Picard iteration]}$$

2. Show that y_1, y_2,.... is a Cauchy sequence, $y^* = \lim_{i\to\infty} y_i$.

3. Conclude that the (unique) limit point y^* satisfies the ODE.

Example: Linear ODEs

- Linear ODE: $\dot{x}(t) = Ax(t)$, $A \in \mathbb{R}^{n \times n}$, with $x_0 = x(t_0)$.
- Picard iteration:

$$\begin{aligned} y_1(t) &= x_0 \\ y_2(t) &= x_0 + \Delta t A x_0 \\ y_3(t) &= x_0 + \Delta t A x_0 + \frac{\Delta t^2}{2} A^2 x_0 \\ &\vdots \end{aligned}$$

  with $\Delta t = t - t_0$.

- Take the limit to get explicit solution

$$x(t) = \sum_{i=0}^{\infty} \frac{1}{i!} [(t - t_0)A]^i x_0 = \exp(A(t - t_0))x_0.$$

Examples for Nonlinear ODEs

- The ODE $\dot{x}(t) = x(t)^2$, with $x(0) = 1$ has th explicit solution

$$x(t) = \frac{1}{1-t} \text{ for } t < 1.$$

Why does the solution not exist for $t \geq 1$?

- The ODE $\dot{x}(t) = 2\sqrt{x}$ with $x(0) = 0$ has more than one solution

$$\text{for example} \quad x(t) = 0 \text{ and } x(t) = t^2.$$

Why is there more than one solution?

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Taylor Expansion of ODEs

A typlor expansion of the solution $x(t)$ can be constructed recursively:

- $x(0) = x_0$
- $\dot{x}(0) = f(x_0)$
- $\ddot{x}(0) = \frac{\partial}{\partial t} f(x(t))\big|_{t_0} = f'(x_0)f(x_0)$
- $\dddot{x}(t) = [f''(x_0) \cdot f(x_0)] \cdot f(x_0) + f'(x_0)f'(x_0)f(x_0)$
- and so on ...
- Finally, $x(t) = x_0 + f(x_0)t + \frac{t^2}{2} f'(x_0)f(x_0) + ...$ for small t.
- **Never work out such expansions by hand!**

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Taylor Expansion of ODEs

A general s-order Taylor expansion can be computed by using AD:

- Set $\phi_0(x) = x$.
- For $i = 0 : s-1$

$$\text{set } \phi_{i+1} = \frac{1}{i+1}\frac{\partial \phi_i}{\partial x}(x) f(x).$$

- Return the Taylor expansion

$$x(t) = \sum_{i=0}^{s} \phi_i(x_0) t^i + \mathbf{O}(t^{s+1}).$$

Integration Algorithm (Constant Step-Size)

Input:

- The right-hand side function f and an initial value x_0.
- Order s and constant step-size $h = \Delta t / N$; set $i = 0$ and $y_0 = x_0$.

Repeat: (until $i = N$)

- Compute $y_{i+1} = \sum_{k=0}^{s} \phi_k(y_i) h^k$ and set $i \leftarrow i + 1$

Theorem: If f is globally Lipschitz continuous and smooth, then

$$\forall\, i \in \{1, ..., N\} \qquad y_i = x(ih) + \mathbf{O}(h^s).$$

Contents

Limitation of Taylor Model Based Integrators

1. Taylor model based intgration is easy to implement, but
   - we need an AD tool (not a big problem)
   - it is not the most efficient scheme for obtaining convergence order s.
2. Runge-Kutta integrators compute an approximation $y \approx x(h)$ by evaluating f at more than one point, but don't evaluate derivatives.

Explicit Runge Kutta Method (Constant Step-size)

Input:

- The right-hand side function f and an initial value x_0.
- Constant step-size $h = \Delta t / N$; set $n = 0$ and $y_0 = x_0$.

Repeat: (unitil $n = N$)

1. Compute iterates $k_i = f(y_n + \sum_{j=1}^{i-1} h a_{i,j} k_j)$ for $i = 1, ..., s$.
2. Set $y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$.

Main idea:

- Choose the coefficients $a_{i,j}$ and b_j such that

$$\forall\, i \in \{1, ..., r\}, \quad \left. \frac{\partial^i y_{n+1}}{\partial h^i} \right|_{h=0} = \phi_i(y_n) \quad \text{(typically } r = s \leq 10\text{)}.$$

Example 1: Euler's Method

- For $s = 1$, the Runge-Kutta method takes the form

$$y_{n+1} = y_n + hb_1 f(y_n).$$

- The first order consistency condition

$$\left.\frac{\partial y_{n+1}}{\partial h}\right|_{h=0} = b_1 f(y_n) = \phi_1(y_n) = f(y_n)$$

  implies that we must choose $b_1 = 1$.

- This gives Euler's method

$$y_{n+1} = y_n + hf(y_n)$$

Example 2: Heun's Method

- Heun's method is given by the coefficient scheme

$$
\begin{array}{cc}
0 & \\
a_{2,1} & 0 \\
\hline
b_1 & b_2
\end{array}
\quad = \quad
\begin{array}{cc}
0 & \\
1 & 0 \\
\hline
\frac{1}{2} & \frac{1}{2}
\end{array}
$$

- The corresponding method can be written as

$$
\begin{aligned}
k_1 &= f(y_n) \\
k_2 &= f(y_n + hk_1) \\
y_{n+1} &= y_n + h\left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right).
\end{aligned}
$$

Example 2: Heun's Method

- The first and second order consistency conditions for $s = 2$ are

$$\left.\frac{\partial y_{n+1}}{\partial h}\right|_{h=0} = (b_1 + b_2) f(y_n) = \phi_1(y_n) = f(y_n)$$

and

$$\left.\frac{\partial^2 y_{n+1}}{\partial h^2}\right|_{h=0} = b_2 a_{2,1} f'(y_n) f(y_n) = \phi_2(y_n) = \frac{1}{2} f'(y_n) f(y_n).$$

- Thus, Heun's method has convergence order $r = 2$, since it satisfies

$$b_1 + b_2 = 1 \quad \text{and} \quad b_2 a_{2,1} = \frac{1}{2}.$$

Example 3: RK4

- A very elegant method of order 4 is given by the scheme

$$
\begin{aligned}
k_1 &= f(y_n) \\
k_2 &= f(y_n + \frac{h}{2} k_1) \\
k_3 &= f(y_n + \frac{h}{2} k_2) \\
k_4 &= f(y_n + h k_3) \\
y_{n+1} &= y_n + h \left(\frac{1}{6} k_1 + \frac{1}{3} k_2 + \frac{1}{3} k_3 + \frac{1}{6} k_4 \right).
\end{aligned}
$$

Implicit Runge Kutta (IRK) Method

- IRK methods are analogous to explicit RK methods, but solve a nonlinear equation system of the form

$$k_i = f\left(y_n + \sum_{j=1}^{s} h a_{i,j} k_j\right)$$

for $i \in \{1, .., s\}$ in order to determine the step

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i.$$