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Norwegian University of Science and Technology

TMA4125 Matematikk 4N

Numerical methods for ordinary differential equations

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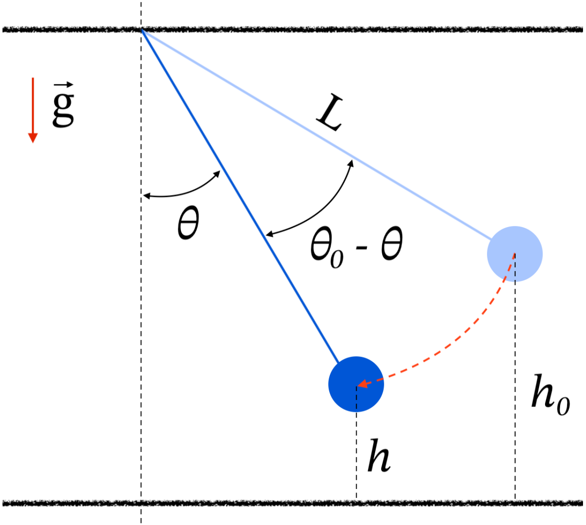
Motivation



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Equation of motion

We want to find $\theta(t)$ fulfilling the following initial value problem:

$$\theta''(t) = -\frac{g}{L}\sin\theta(t),$$
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For angles larger than 5° this is very inaccurate!

Introduction

First-order ODEs

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$$H_2O_2 + 3I^- + 2H^+ \xrightarrow{k_1} I_3^- + 2H_2O$$
$$I_3^- + 2S_2O_3^{2-} \xrightarrow{k_2} 3I^- + S_4O_6^{2-}$$

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Rate laws:

$$x' = -k_1 x^3 + 3k_2 y z^2$$
$$y' = k_1 x^3 - k_2 y z^2$$
$$z' = -k_2 y z^2$$

Introduction: higher-order ODEs

Pendulum equation

$$\theta''(t) = -k \sin\theta(t), \quad \theta(0) = \theta_0, \quad \theta'(0) = 0$$

Let's rewrite this equation:

Euler's method

$$\boldsymbol{y}'(t_n) = \boldsymbol{f}(t_n, \boldsymbol{y}(t_n))$$

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Approximating the derivative:

$$\boldsymbol{y}' \approx \frac{\Delta \boldsymbol{y}}{\Delta t}, \quad \text{that is,} \quad \boldsymbol{y}'(t_n) \approx \frac{1}{h}\left[\boldsymbol{y}(t_{n+1}) - \boldsymbol{y}(t_n)\right]$$

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This gives us Euler's method:

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\boldsymbol{f}(t_n, \boldsymbol{y}_n)$$

$n = 0:$

$n = 1:$

$\vdots$

Euler's method: example

$$y' = \underbrace{2 + 2^{-t} - \sin(0.25\pi y)}_{=f(t,y)}, \quad y(0) = 2$$

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Issue: we would need $\boldsymbol{y}_{n+1}$ to compute $\boldsymbol{y}_{n+1}$ $\rightarrow$ **implicit** method!

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This gives us **Heun's method**:

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First step:

- Evaluate $f(t_0, y_0)$
- Compute Euler step: $y_1^{\text{Euler}} = y_0 + hf(t_0, y_0)$
- Evaluate $f(t_1, y_1^{\text{Euler}})$
- Compute $y_1 = y_0 + \frac{h}{2}\left[f(t_0, y_0) + f(t_1, y_1^{\text{Euler}})\right]$

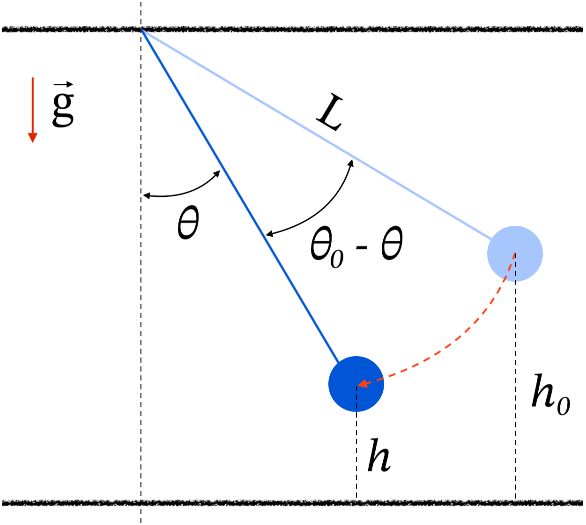
Heun's method: example

$$y' = 2 + 2^{-t} - \sin(0.25\pi y), \quad y_1 = 3, \quad h = 0.5$$

Second step:

- Evaluate $f(t_1, y_1)$
- Compute Euler step: $y_2^{\text{Euler}} = y_1 + hf(t_1, y_1)$
- Evaluate $f(t_2, y_2^{\text{Euler}})$
- Compute $y_2 = y_1 + \frac{h}{2}\left[f(t_1, y_1) + f(t_2, y_2^{\text{Euler}})\right]$

Exercise



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If y is smooth enough, we can write the Taylor expansion:

$$y(t_n + h) = y(t_n) + hy'(t_n) + \frac{h^2}{2!}y''(t_n) + \frac{h^3}{3!}y'''(t_n) + \ldots$$

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- First order: $y_{n+1} = y_n + hy'(t_n) = y_n + hf(t_n, y_n)$ $\rightarrow$ **Euler's method!**
- Second order: $y_{n+1} = y_n + hy'(t_n) + \frac{h^2}{2}y''(t_n) = ?$

Taylor method of second order

$$y_{n+1} = y_n + hy'(t_n) + \frac{h^2}{2}y''(t_n)$$

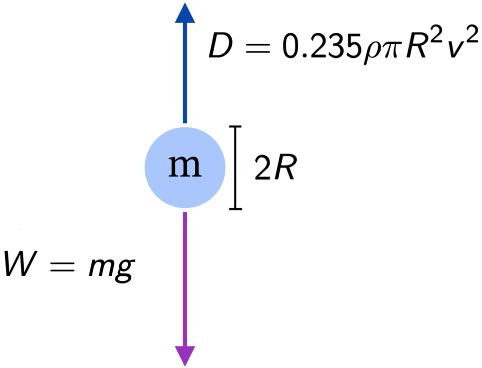
Taylor method of second order: example

$$y' = 2 + \mathrm{e}^{-t}y \quad y(0) = 1, \quad h = 0.25$$

Algorithm:

$$y_{n+1} = y_n + hf(t_n, y_n) + \frac{h^2}{2}\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\Bigg|_{(t_n, y_n)}$$

Accuracy test: sphere in free fall



One-step methods

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h_n \underbrace{\boldsymbol{\Phi}(t_n, \boldsymbol{y}_n, \boldsymbol{y}_{n+1}, h_n)}_{\text{increment function}}$$

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Consistency error

$$\varepsilon_n = \left| \frac{\boldsymbol{y}(t_n + h) - \boldsymbol{y}(t_n)}{h} - \boldsymbol{\Phi}(t_n, \boldsymbol{y}(t_n), \boldsymbol{y}(t_n + h), h) \right|$$

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If $\varepsilon_n \leq C h^p$ for $h \to 0$ $\Rightarrow$ order p consistency

Consistency

Euler's method

$$\varepsilon_n = \left| \frac{y(t_n + h) - y(t_n)}{h} - f(t_n, y(t_n)) \right|$$

Consistency

Second-order Taylor method

$$\varepsilon_n = \left| \frac{y(t_n + h) - y(t_n)}{h} - \left[f(t_n, y(t_n)) + \frac{h}{2} \frac{\mathrm{d}f}{\mathrm{d}t} \right] \right|$$

Consistency

Heun's method

$$\varepsilon_n = \left| \frac{y(t_n + h) - y(t_n)}{h} - \frac{f(t_n, y(t_n)) + f(t_n + h, y(t_n) + hf(t_n, y(t_n)))}{2} \right|$$

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$$y(t_n + h) - y(t_n) = hy'(t_n) + \tfrac{h^2}{2} y''(t_n) + \tfrac{h^3}{6} y'''(\xi_n), \quad t_n \le \xi_n \le t_n + h$$

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$$f(t + h, y + \delta) = f + h\frac{\partial f}{\partial t} + \delta \frac{\partial f}{\partial y} + \frac{1}{2!} \left[h^2 \frac{\partial^2 f}{\partial t^2} + \delta^2 \frac{\partial^2 f}{\partial y^2} + 2h\delta \frac{\partial^2 f}{\partial y \partial t} \right] \Big|_{(\tau,\zeta)}$$

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$$\varepsilon_n = \left| y'(t_n) - f(t_n, y(t_n)) + \frac{h}{2}\left[y'' - \left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\right]\Bigg|_{(t_n, y(t_n))} + (\dots)h^2 \right|$$

Consistency

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$$\varepsilon_n = \left| \frac{y(t_n+h)-y(t_n)}{h} - \frac{f(t_n,y(t_n)) + f(t_n+h, y(t_n)+hf(t_n,y(t_n)))}{2} \right|$$

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$$\varepsilon_n = \mathcal{O}(h^2)$$

Convergence

Remember the definition of the consistency error:

$$\varepsilon_n = \left| \frac{\boldsymbol{y}(t_n + h) - \boldsymbol{y}(t_n)}{h} - \boldsymbol{\Phi}(t_n, \boldsymbol{y}(t_n), \boldsymbol{y}(t_n + h), h) \right|$$

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$$\epsilon_g = \max_{n=1,2,\ldots,N} |\boldsymbol{y}_n - \boldsymbol{y}(t_n)|$$

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Question

If a one-step method is consistent of order p,
does it also converge with that order**?**

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Question

If a one-step method is consistent of order p,
does it also converge with that order**?**

Not necessarily!

Convergence

Theorem

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Consistency of order p

$+$

Lipschitz continuity

$=$

Convergence of order p

Convergence

$$\epsilon_g \leq Ch^p$$

How do we interpret this inequality?

Lipschitz continuity

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$$

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Important: all continuously differentiable functions are *also* Lipschitz

Lipschitz continuity

Example: $f(t, y) = t + |y|$

Lipschitz continuity

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Triangle inequality: $|\boldsymbol{a} + \boldsymbol{b}| \leq |\boldsymbol{a}| + |\boldsymbol{b}|$

Lipschitz continuity: Euler's method

In general, we want to know if the increment function inherits the Lipschitz continuity from the right-hand side function!

Increment function: $\boldsymbol{\Phi}(t, \boldsymbol{y}, h) = \boldsymbol{f}(t, \boldsymbol{y})$

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Assumption: $\boldsymbol{f}(t, \boldsymbol{y})$ is Lipschitz continuous:

$$|\boldsymbol{f}(t, \boldsymbol{x}) - \boldsymbol{f}(t, \boldsymbol{z})| \leq L\,|\boldsymbol{x} - \boldsymbol{z}| \quad \text{for all} \quad (t, h, \boldsymbol{x}, \boldsymbol{z})$$

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$\Rightarrow$ Therefore, since we've already seen that
Euler's method is first-order consistent,
then it will also be **first-order convergent**
if $\boldsymbol{f}$ is Lipschitz!

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Lipschitz continuity: Heun's method

$$\boldsymbol{\Phi}(t, \boldsymbol{y}, h) = \frac{1}{2}\left[\boldsymbol{f}(t, \boldsymbol{y}) + \boldsymbol{f}(t + h, \boldsymbol{y} + h\boldsymbol{f}(t, \boldsymbol{y}))\right]$$

Lipschitz continuity: Heun's method

$$\boldsymbol{\Phi}(t, \boldsymbol{y}, h) = \frac{1}{2}\left[\boldsymbol{f}(t, \boldsymbol{y}) + \boldsymbol{f}(t+h, \boldsymbol{y} + h\boldsymbol{f}(t, \boldsymbol{y}))\right] \;\Rightarrow\; |\boldsymbol{\Phi}(t, \boldsymbol{x}, h) - \boldsymbol{\Phi}(t, \boldsymbol{z}, h)|$$

$$= \frac{1}{2}\left|\left[\boldsymbol{f}(t, \boldsymbol{x}) + \boldsymbol{f}(\underbrace{t+h}_{\tilde{t}}, \underbrace{\boldsymbol{x} + h\boldsymbol{f}(t, \boldsymbol{x})}_{\tilde{\boldsymbol{x}}})\right] - \left[\boldsymbol{f}(t, \boldsymbol{z}) + \boldsymbol{f}(\underbrace{t+h}_{\tilde{t}}, \underbrace{\boldsymbol{z} + h\boldsymbol{f}(t, \boldsymbol{z})}_{\tilde{\boldsymbol{z}}})\right]\right|$$

Lipschitz continuity: Heun's method

Convergence (?) study

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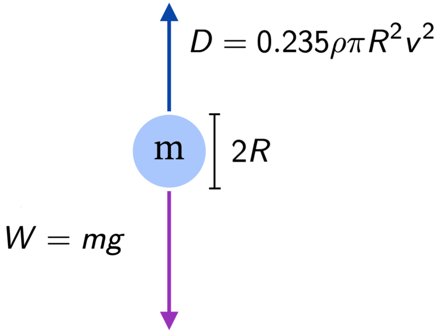
Problem 1



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Exact solution:

$$v(t) = 3.3\tanh(2.9725t)$$

Convergence (?) study

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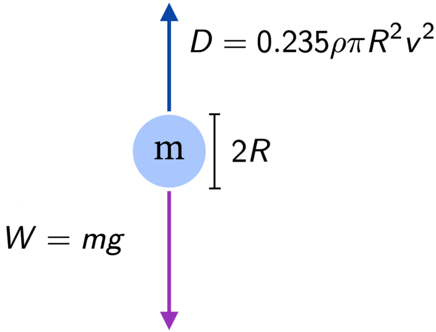

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$$y'(t) = 2\sqrt{y}, \quad y(0) = 0$$

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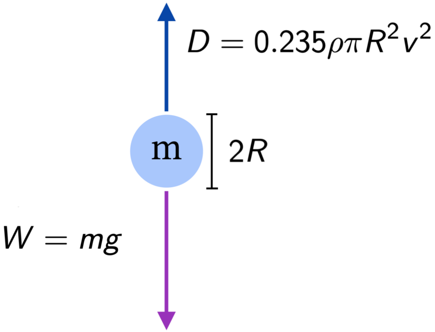

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Issue: Lipschitz condition violated for $y = 0$