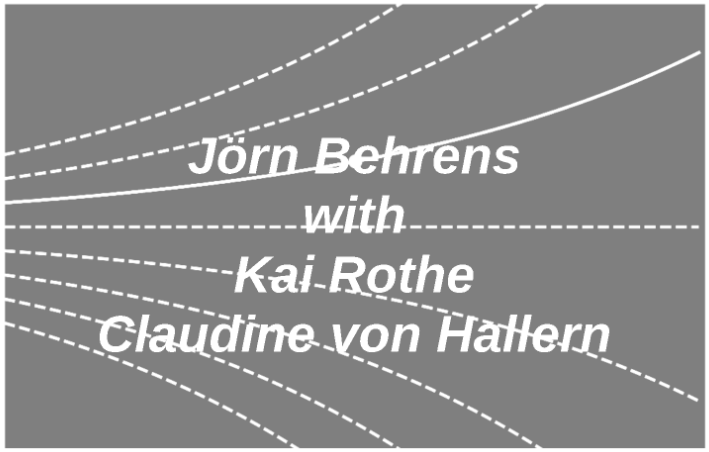
Differential Equations I



Numerical Methods

Chapter 6.10

Introduction

Motivation:

- By now we know a number of analytical solution techniques. What if the ODE is too complicated?
- With the mathematical tool set, we may be able to state the solvability, but we may not be able to actually solve.
- Idea: Find an (approximate) solution by means of numerical methods!

Idea:

- Consider ODE of 1st order:

$$y'(x) = f(x, y(x))$$

- Let initial conditions be

$$y(x_0) = y_0$$

- Observation: In (x_0, y_0) the slope $y'(x_0) = F(x_0, y_0)$ of the solution function y is known!
- Idea: Approximate solution by means of the tangent line (linearization).

Method: (Euler's Integration Method)

- Consider the initial value problem of 1st order:

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0$$

- Define equidistant nodes with increment h:

$$x_k = x_0 + kh \quad (k = 1, 2, \ldots).$$

- Then one obtains an approximation y_k to the exakt solution values $y(x_k)$ by

$$y_{k+1} = y_k + hf(x_k, y_k), \quad k = 0, 1, 2, \ldots$$

- This method is called Euler's integration method.
  Other names: *polygon method, Euler's method*.

Remarks:

- Euler's method can only be used with very small increments h.
- The method is the simplest *explicit one-step method*.

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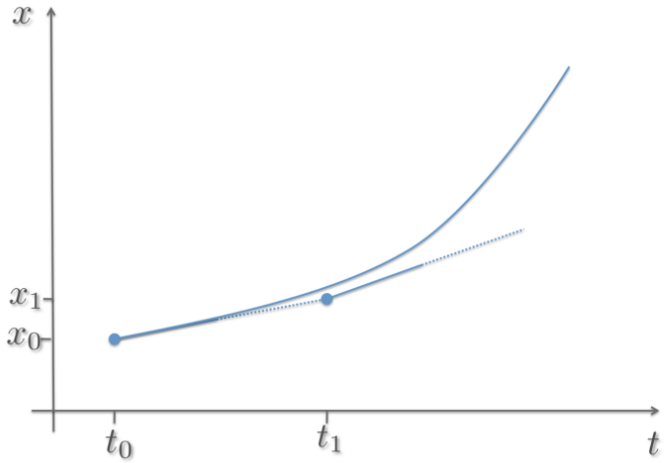

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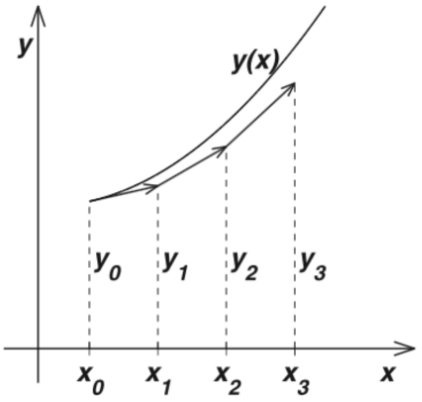

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Discretization Error

Notation:

- Use a general (implicit) form of the calculation rule

$$y_{k+1} = y_k + h\Phi(x_k, y_k, y_{k+1}, h).$$

- If Φ depends only on x_k, y_k and h, then an explicit rule is given.
- If Φ also depends on y_{k+1}, then in general in each (time) step a non-linear equation needs to be solved (*implicitly*).
- Example: Euler's method uses $\Phi(x_k, y_k, y_{k+1}, h) = f(x_k, y_k)$.

Definition: (Lokal Discretization Error)
The lokal discretization error at x_{k+1} is defined by

$$d_{k+1} := y(x_{k+1}) - y(x_k) - h\Phi(x_k, y(x_k), y(x_{k+1}), h).$$

Remark: This is the error compared to the exact solution, generated within one sigle step $x_k \to x_{k+1}$.

Definition: (Order of Error)
A one-step method $y_{k+1} = y_k + h\Phi(x_k, y_k, y_{k+1}, h)$ has an order of error p, if for the lokal discretization error d_k it holds:

$$\max_{1 \le k \le n} |d_k| \le D = \text{const.} \cdot h^{p+1} = \mathcal{O}(h^{p+1}).$$

Proposition: (Estimation of the Global Discretization Error)
For the global error g_n at a fixed position $x_n = x_0 + nh$ we have

- For an explicit one-step method:

$$|g_n| \le \frac{D}{hL}\left(e^{nhL} - 1\right) \le \frac{D}{hL} e^{nhL}.$$

- For an implicit method:

$$|g_n| \le \frac{D}{hK(1-hL)}\left(e^{nhL} - 1\right) \le \frac{D}{hK(1-hL)} e^{nhL}.$$

Here D is an upper bound for the local discretization error, L a (Lipschitz-) constant depending on the rule Φ, and K a constant.

Remarks:

- For solution functions with suitable properties (e.g. two times cont. differentiable) one shows $D \le \frac{1}{2}h^2M$, where M is an upper bound for y''.
- For Euler's method this yields:

$$|g_n| \le h\frac{M}{2L}e^{L(x_n - x_0)} =: hC, \quad C \in \mathbb{R}.$$

- Interpretation: For fixed position x_n and decreasing increment $h = \frac{x_n - x_0}{n}$ (therefore increasing n) the global discretization error decreases proportional to the increment.

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Remark: This is the error compared to the exact solution, generated within one sigle step $x_k \to x_{k+1}$.

Definition: (Global Discretization Error)
The global discretization error at x_k is defined by

$$g_k := y(x_k) - y_k.$$

Remark: This is the error between the exact solution $y(x_k)$ and and the numerically computed solution y_k.

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For the global error g_n at a fixed position $x_n = x_0 + nh$ we have

- For an explicit one-step method:

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Corollary:
The global discretization error g_n of an explicit method with order p is bounded by

$$|g_k| \leq \frac{\text{const.}}{L} e^{nhL} \cdot h^p = \mathcal{O}(h^p).$$

Trapeziodal Method

Idea: (Method from Richardson-Extrapolation)

- Goal: Method of order $p > 1$.
- Compute y_h with increment $h_1 = h$ and the same position y_{2h} with $h_2 = \frac{h}{2}$, obtain

$$\begin{aligned} y_h &\approx y(x) + c_1 h + \mathcal{O}(h^2) \\ y_{2h} &\approx y(x) + c_1 \frac{h}{2} + \mathcal{O}(h^2) \end{aligned}$$

- Richardson-Extrapolation yields

$$\tilde{y} = 2y_{2h} - y_h \approx y(x) + \mathcal{O}(h^2).$$

Developement: (Improved Polygonal Method)

- Instead of applying Richardson-Extrapolation to result of two polygonal methods (PM), apply extrapolation in each step!
- **Normal Step**: PM with h.

$$y_{k+1}^{(1)} = y_k + hf(x_k, y_k)$$

- **Double Step**: PM executed twice with $\frac{h}{2}$:

$$\begin{aligned} y_{k+1}^{(2)} &= y_k + \tfrac{h}{2} f(x_k, y_k) \\ y_{k+1}^{(2)} &= y_{k+\frac{1}{2}}^{(2)} + \tfrac{h}{2} f(x_k + \tfrac{h}{2}, y_{k+\frac{1}{2}}^{(2)}) \end{aligned}$$

- **Richardson-Extrapolation**:

$$\begin{aligned} y_{k+1} &= 2y_{k+1}^{(2)} - y_{k+1}^{(1)} \\ &= 2y_{k+\frac{1}{2}}^{(2)} + hf(x_k + \tfrac{h}{2}, y_{k+\frac{1}{2}}^{(2)}) - y_k - hf(x_k, y_k) \\ &= 2y_k + hf(x_k, y_k) + hf(x_k + \tfrac{h}{2}, y_{k+\frac{1}{2}}^{(2)}) - y_k - hf(x_k, y_k) \\ &= y_k + hf(x_k + \tfrac{h}{2}, y_k + \tfrac{h}{2} f(x_k, y_k)). \end{aligned}$$

Idea: (Heun's Method)

- Iterate only one step of the fixed point iteration:

$$\begin{aligned} y_{k+1}^{(1)} &= y_k + f(x_k, y_k) \\ y_{k+1} &= y_k + \frac{h}{2} \left[f(x_k, y_k) + f(x_{k+1}, y_{k+1}^{(1)}) \right]. \end{aligned}$$

- This means Euler's method determines predictor value $y_{k+1}^{(1)}$, trapezoidal method determins corrected value y_{k+1}.
- The following Heun's method is a predictor-corrector method:

$$\begin{aligned} k_1 &= f(x_k, y_k) \\ k_2 &= f(x_k + h, y_k + hk_1) \\ y_{k+1} &= y_k + \frac{h}{2} k_1 + k_2 \end{aligned}$$

Algorithm: (Improved Polygonal Method)

$$\begin{aligned} k_1 &= f(x_k, y_k) \\ k_2 &= f(x_k + \frac{h}{2}, y_k + \frac{h}{2} k_1) \\ y_{k+1} &= y_k + h k_2 \end{aligned}$$

Remark: The improved polygonal method uses

$$\Phi(x_k, y_k, y_{k+1}, h) = f(x_k + \frac{h}{2}, y_k + \frac{h}{2} f(x_k, y_k)).$$

Idea: (Trapezoidal Method)

- New Idea: Integrate the ODE $y'(x) = f(x, y(x))$ for one time step and obtain

$$y(x_{k+1}) - y(x_k) = \int_{x_k}^{x_{k+1}} f(x, y(x)) \, dx$$

- Solve the integral by a (numerical) quadrature rule (here trapezoidal rule):

$$y_{k+1} = y_k + \frac{h}{2} \left[f(x_k, y_k) + f(x_{k+1}, y_{k+1}) \right]$$

- Obtain an implicit method, called trapezoidal method.

Remarks: (Trapezoidal Method)

- Since the implicit solution often involves a non-lineare problem, solve by fixed point iteration:

$$\begin{aligned} y_{k+1}^{(0)} &= y_k + f(x_k, y_k) \\ y_{k+1}^{(s+1)} &= y_k + \frac{h}{2} \left[f(x_k, y_k) + f(x_{k+1}, y_{k+1}^{(s)}) \right] \quad s = 0, 1, 2, \ldots \end{aligned}$$

- Obtain convergence, if $|f(x, y) - f(x, y^*)| \leq L|y - y^*|$ (Lipschitz continuous) and $\frac{hL}{2} < 1$ (Banach's Fixed Point Theorem).

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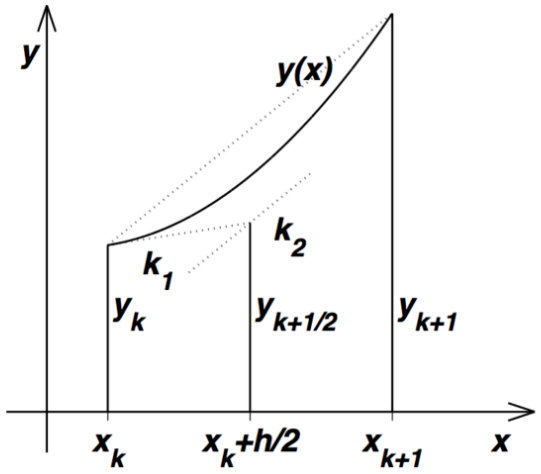

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Runge-Kutta Methods

Preliminary Remarks:

- Heun's method and the improved polygonal method are both examples of explicit two-stage Runge-Kutta methods of order 2.
- For the description of Runge-Kutta methods of higher order we start from the integral equation

$$y(x_{k+1}) - y(x_k) = \int_{x_k}^{x_{k+1}} f(x, y(x))\, dx.$$

- For solving the integral use a general quadrature rule with 3 nodes in the interval $[x_k, x_{k+1}]$. This yields the ansatz:

$$y_{k+1} = y_k + h[c_1 f(\xi_1, y(\xi_1)) + c_2 f(\xi_2, y(\xi_2)) + c_3 f(\xi_3, y(\xi_3))].$$

- Here let $c_1 + c_2 + c_3 = 1$, ξ_i be the nodes.

Determination of Nodes and Values:

- Use the nodes

$$\xi_1 = x_k, \quad \xi_2 = x_k + a_2 h, \quad \xi_3 = x_k + a_3 h, \quad 0 < a_2, a_3 \leq 1.$$

- Since $\xi_1 = x_k$ we have $y(\xi_1) = y_k$.
- For $y(\xi_2)$ and $y(\xi_3)$ utilize predictor approach:

$$\begin{array}{rcl} y(\xi_2): & y_2^* & = y_k + h b_{11} f(x_k, y_k) \\ y(\xi_3): & y_3^* & = y_k + h b_{11} f(x_k, y_k) + h b_{22} f(x_k + a_2 h, y_2^*). \end{array}$$

- One obtains parameters $a_2, a_3, b_{21}, b_{31}, b_{32}, c_1, c_2, c_3$, to be chosen such that an optimal order of error is achieved.

Algorithm: (3-Stage Runge-Kutta Method)

$$\begin{array}{rcl} k_1 & = & f(x_k, y_k) \\ k_2 & = & f(x_k + a_2 h, y_k + h b_{21} k_1) \\ k_3 & = & f(x_k + a_3 h, y_k + h(b_{31} k_1 + b_{32} k_2)) \\ y_{k+1} & = & y_k + h[c_1 k_1 + c_2 k_2 + c_3 k_3]. \end{array}$$

Example: Heun's Method of 3rd order is given by the following parameters:

$$a_1 = \frac{1}{3},\ a_2 = \frac{2}{3},\ c_1 = \frac{1}{4},\ c_2 = 0,\ c_3 = \frac{3}{4}, b_{32} = \frac{2}{3}, b_{31} = a_3 - b_{32} = 0.$$

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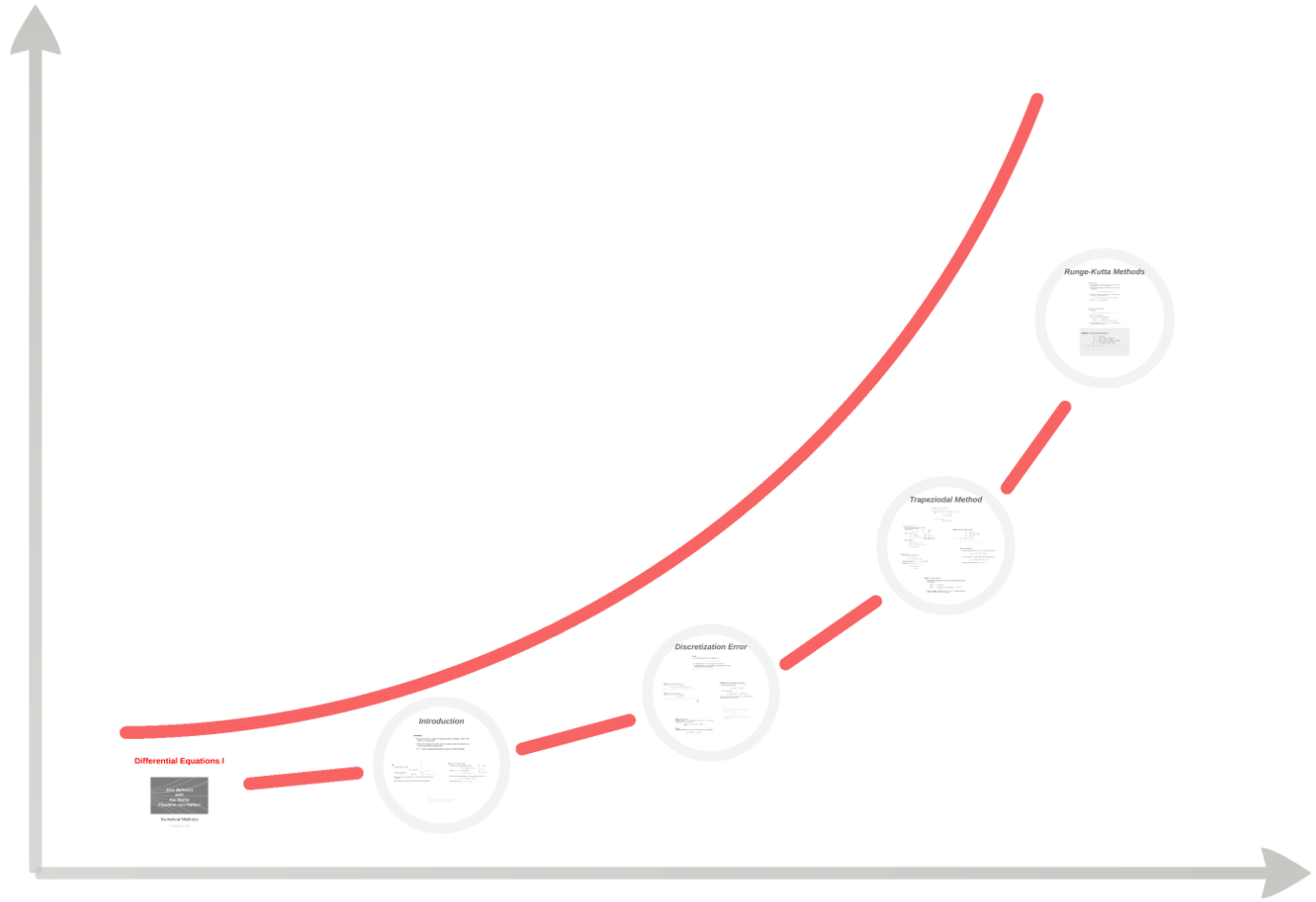
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