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Fachbereich C – Mathematik und Naturwissenschaften
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Numerical Analysis and Simulation I: Ordinary Differential Equations (ODEs)

Sheet 4 - Runge-Kutta Methods and Step Size Control

Return of the Exercise Sheet: Tuesday, November 18th before the lecture

Exercise 7: *Formulation of Runge-Kutta-Methods*
For solving the IVP $y' = f(x, y)$, $y(x_0) = y_0$ ($y : \mathbb{R} \to \mathbb{R}^n$) numerically, the formula of a general Runge-Kutta method with s stages reads

$$\begin{aligned} y(x+h) &\doteq y_0 + h \sum_{i=1}^{s} b_i k_i \\ k_i &= f(x_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j), \quad i = 1, \ldots, s \end{aligned}$$

for given coefficients c_i, b_i, a_{ij}. Another formulation using the same coefficients is

$$\begin{aligned} y(x+h) &\doteq y_0 + h \sum_{i=1}^{s} b_i f\left(x_0 + c_i h, y_i\right) \\ y_i &= y_0 + h \sum_{j=1}^{s} a_{ij} f\left(x_0 + c_j h, y_j\right), \quad i = 1, \ldots, s. \end{aligned}$$

a) Show that the two formulations are equivalent, i.e. they produce the same approximation.

a) What is the meaning of the values k_i in comparison to the y_i ?

Exercise 8: *Simple Embedded Schemes*
For the numerical treatment of the initial value problem (IVP) $y' = f(x, y)$, $y(x_0) = y_0$, we consider the embedded Runge-Kutta (RK) method

$$y_1 = y_0 + hK_1 \quad \text{and} \quad \hat{y}_1 = y_0 + h/2(K_1 + K_2)$$

with increments

$$\begin{aligned} K_1 &= f(x_0, y_0) \\ K_2 &= f(x_0 + h, y_0 + hK_1). \end{aligned}$$

a) State the corresponding Butcher tableaus. Verify that y_1 defines a method of order 1 and $\hat{y}_1$ a method of order 2.

b) How many function evaluations of the right-hand side $f(x, y)$ are necessary for this method (per step)? Which approximation y_1 or $\hat{y}_1$ is used to go on with computations? Please argue.

c) Sketch an algorithm for the numerical approximation of an IVP applying the given method and including step size control.

Exercise 9: *Step-Size Control*
Consider the scalar IVP $y'(x) = f(x, y(x))\,,\ x \in [0, b],\ y(0) = y_0$ with a sufficiently smooth right-hand side $f : [0, b] \times \mathbb{R} \to \mathbb{R}$. Approximations y_n to $y(x_n)$ should be computed by means of the *second order Collatz method* with variable step size

$$\begin{aligned} y_{n+1} &= y_n + h_n k_2\,, \\ k_1 &= f(x_n, y_n)\,, \\ k_2 &= f(x_n + \tfrac{1}{2}h_n, y_n + \tfrac{1}{2}h_n k_1)\,. \end{aligned}$$

Kutta's third order rule

$$\begin{aligned} \hat{y}_{n+1} &= y_n + \frac{1}{6}h_n(k_1 + 4k_2 + k_3)\,, \\ k_1 &= f(x_n, y_n)\,, \\ k_2 &= f(x_n + \tfrac{1}{2}h_n, y_n + \tfrac{1}{2}h_n k_1)\,, \\ k_3 &= f(x_n + h_n, y_n - h_n k_1 + 2h_n k_2) \end{aligned}$$

should be used to be able to perform a step size control .

a) State the Butcher-Tableaus for both methods.

b) Estimate the local discretisation error τ_{n+1} for the Collatz method. (You can just give a short formula $\tau_{n+1} \approx e_{n+1} = \dots$)

c) Let TOL_n be a given tolerance for the local error in this step. What would have been an optimal step size $h_{n,\mathrm{opt}}$ with respect to the given tolerance? Why? Sketch an algorithm with step size control!

d) How many evaluations of the right-hand side are necessary to compute the new approximation y_{n+1} together with a suggestion for the next step size h_{n+1} ?

Homework 7: *Step size control with* `ATOL` *and* `RTOL` (10 Points)
Integration codes using step size control require the assignment of absolute and relative tolerances: `ATOL` and `RTOL`, respectively. Based on an estimate of the local error e^{loc}, we demand

$$|e_i^{\mathrm{loc}}| \le \mathtt{ATOL} + WT_i \cdot \mathtt{RTOL}, \quad WT_i = \max(|y_{0i}|, |y_{1i}|) \qquad (\star)$$

for all vector components $i = 1, \dots, n$. Here,

$$y_0 = (y_{01}, y_{02}, \dots, y_{0n})^\top \quad \text{and} \quad y_1 = (y_{11}, y_{12}, \dots, y_{1n})^\top$$

denote the previously and newly computed approximation.

a) Let $y_0 = (500, 0.005)^\top, y_1 = (499, 0.008)^\top, e^{\mathrm{loc}} = (3, 0.005)^\top$ be given. For which of the 4 combinations of `ATOL`$= 0$, `ATOL`$= 0.01$ and `RTOL`$= 0$, `RTOL`$= 0.01$ is the criterion $(\star)$ fulfilled?

b) For the step size control, one introduces the quantity

$$\mathrm{ERR} := \sqrt{\frac{1}{n}\sum_{j=1}^{n}\left(\frac{e_j^{\mathrm{loc}}}{\mathtt{ATOL} + WT_j \cdot \mathtt{RTOL}}\right)^2}\,.$$

Let the condition $(\star)$ be fulfilled for all components. We assume `ATOL` $\neq 0$. Which property follows for ERR? For which value of ERR do we get an optimal step size (w.r.t. the given tolerances)?

c) Let y_1 and $\hat{y}_1$ be numerical approximations of order p and $p + 1$, respectively. Formulate an algorithm for the calculation of the optimal step size based on ERR using the (only necessary) criterion obtained in part (b).

Homework 8: *Runge-Kutta-Fehlberg 1(2)* (10 Points)
Our aim is to solve the ODE-IVP $y' = f(x, y),\ y(x_0) = y_0$ numerically including a step size control. For this purpose, we use an embedded scheme based on explicit Runge-Kutta methods with $s = 3$ stages. The corresponding Butcher tableau reads:

$$\begin{array}{c|ccc} c_1 & 0 & 0 & 0 \\ c_2 & a_{21} & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 \\ \hline & b_1 & b_2 & 0 \\ \hline & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 \end{array}$$

The corresponding approximations are

$$\begin{aligned} y_1 &= y_0 + h\big(b_1 k_1 + b_2 k_2\big), \\ \hat{y}_1 &= y_0 + h\big(\hat{b}_1 k_1 + \hat{b}_2 k_2 + \hat{b} k_3\big), \end{aligned}$$

with the increments k_1, k_2, k_3.

a) How many function evaluations are required in each step to calculate the approximations y_1 and $\hat{y}_1$?

b) Choose the coefficients c_3, a_{31}, a_{32} (possibly in dependence on the other parameters) such that the function evaluation $f(x_0 + c_3 h, z_3)$ of one step coincides with the function evaluation $f(x_0, y_0)$ in the subsequent step. This technique is called FSAL (first same as last) and saves one function evaluation.

c) Formulate the conditions such that y_1 and $\hat{y}_1$ become consistent approximations of order 1 and 2, respectively. Determine a set of coefficients satisfying these order conditions and the conditions from part (b) as well as the fundamental property

$$c_i = \sum_{j=1}^{3} a_{ij} \qquad \text{for each } \ i = 1, 2, 3.$$

(A feasible set of coefficients is not unique here. Try to find the free parameters.)