Fachbereich Mathematik **WiSe 2012/2013**
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Numerik steifer Probleme

Aufgabenblatt 5

Aufgabe 1

The MATLAB solver `ode23s` is based on a so-called Rosenbrock formula. For an autonomous system of ODEs $\dot{\mathbf{y}}(t) = \mathbf{f}(\mathbf{y}(t))$ the basic method is defined by

$$\begin{aligned} (\mathbf{I} - a\Delta t\mathbf{J})\,\mathbf{k}_1 &= \mathbf{f}\,(\mathbf{y}_n)\,, \\ (\mathbf{I} - a\Delta t\mathbf{J})\,\mathbf{k}_2 &= \mathbf{f}\left(\mathbf{y}_n + \frac{1}{2}\Delta t\mathbf{k}_1\right) - a\Delta t\mathbf{J}\mathbf{k}_1, \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + \Delta t\mathbf{k}_2, \end{aligned}$$

where $a = 1/\left(2+\sqrt{2}\right)$ and $\mathbf{J} = \frac{\partial \mathbf{f}(\mathbf{y}_n)}{\partial \mathbf{y}}$. Show that this method is consistent of second order.

Hint: For $0 < \Delta t < 1/(2a\|\mathbf{J}\|_2)$ consider the solution $\mathbf{k}$ of the linear system

$$(\mathbf{I} - a\Delta t\mathbf{J})\mathbf{k} = \mathbf{f}.$$

Now, first show $\|\mathbf{k}\|_2 \leq 2\|\mathbf{f}\|_2$. Then use Taylor expansion for $\mathbf{k}_1, \mathbf{k}_2$ and $\mathbf{y}_{n+1}$.

Do you actually need $\mathbf{J} = \frac{\partial \mathbf{f}(\mathbf{y}_n)}{\partial \mathbf{y}}$ in your proof or would an approximation $\mathbf{J}$ of the Jacobian still lead to a method of second order? (4 P)

Aufgabe 2

Prove the first two assertions of Lemma 3:

Assume the standard assumptions hold. Then there is $\delta > 0$ such that for all $x \in B(\delta)$:

a) $\|F'(x)\| \leq 2\|F'(x^*)\|$,

b) $\|F'(x)^{-1}\| \leq 2\|F'(x^*)^{-1}\|$

Hint: Use the Banach Lemma: If $\mathbf{M} \in \mathbb{R}^{n\times n}$ with $\|\mathbf{M}\| < 1$, then $\mathbf{I} - \mathbf{M}$ is nonsingular and

$$\|(\mathbf{I} - \mathbf{M})^{-1}\| \leq \frac{1}{1 - \|\mathbf{M}\|}.$$

(4 P)

Aufgabe 3

Consider the model of Field, Koros and Noyes for the Orego problem:

$$\dot{c} = \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \end{pmatrix} = \begin{pmatrix} s(c_2 - c_1c_2 + c_1 - qc_1^2) \\ \frac{1}{s}(-c_2 - c_1c_2 + c_3) \\ w(c_1 - c_3) \end{pmatrix},$$

with $s = 77.27$, $w = 0.161$ and $q = 8.375 \cdot 10^{-6}$ and initial values $c_1(0) = 1$, $c_2(0) = 2$ and $c_3(0) = 3$, $t \in (0, 360]$. For those interested: c_1 corresponds to $HBrO_2$, c_2 to Bromide ions and c_3 to $Ce(IV)$.

From http://pitagora.dm.uniba.it/˜testset/problems/orego.php : The OREGO problem originates from the celebrated Belousov Zhabotinskii (BZ) reaction. When certain reactans, like bromous acid, bromide ion and cerium ion, are combined, they exhibit a chemical reaction which, after an induction period of inactivity, oscillates with change in structure and in color, from red to blue and viceversa. The color changes are caused by alternating oxidationreductions in which the cerium switches its oxidation state from Ce(III) to Ce(IV).

Solve this problem using the time adaptive method of Cash with a relative and absolute tolerance of 10^{-4}.

$$\begin{array}{c|ccc}
\gamma & \gamma & 0 & 0 \\
\delta & \tau-\gamma & \gamma & 0 \\
1 & \alpha & \beta & \gamma \\
\hline
b_i & \alpha & \beta & \gamma \\
\hat{b}_i & \hat{\alpha} & \hat{\beta} & 0
\end{array}$$

Tabelle 1: Butcher array for the method of Cash; $\alpha = 1.2084966491760101$, $\beta = -0.6443631706844691$, $\gamma = 0.4358665215084580$, $\delta = 0.7179332607542295$, $\tau - \gamma = 0.2820667392457705$, $\hat{\alpha} = 0.7726301276675511$ and $\hat{\beta} = 0.2273698723324489$.

To solve the nonlinear equation systems, program a Newton iteration and try to come up with a reasonable termination criterion for that. To compare your solutions, look at the website mentioned and use the reference final values: $c_1(360) = 1.0008149$, $c_2(360) = 1228.1785$ and $c_3(360) = 132.05549$. (4 P)

Abgabe: Montag, 26.11.2012, in der Vorlesung