Exercise sheet no. 7 – Numerics for instationary differential equations

Exercise 20:

Let V be a separable Hilbert space with norm $\|\cdot\|$ and corresponding inner product (\cdot,\cdot) .

Prove: For a sequence of Fourier coefficients $\{u_n\}_n \subset V$ defined by

$$u_n = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\varphi} \widehat{u}(\varphi) d\varphi, \qquad \widehat{u}(\varphi) = \sum_{n=0}^{\infty} u_n e^{in\varphi}$$

Parseval's theorem holds:

$$\sum_{n=0}^{\infty} ||u_n||^2 = \frac{1}{2\pi} \int_0^{2\pi} ||\widehat{u}(\varphi)||^2 d\varphi.$$

Exercise 21: (Adaptive step sizes for Runge–Kutta-Methods)

For adaptive step sizes one uses embedded methods of the form

$$\widehat{y}_1 = y_0 + h\left(\widehat{b}_0 f(t_0, y_0) + \sum_{j=1}^s \widehat{b}_j Y_j'\right) = y_0 + \left(h\widehat{b}_0 f(t_0, y_0) + \sum_{j=1}^s \widehat{d}_j Z_j\right)$$

with the same nodes c_i but of lower order (for Radau: order s). Hence, we have

$$\widehat{y}_1 - y_1 = h\widehat{b}_0 f(t_0, y_0) + \sum_{j=1}^s h(\widehat{b}_j - b_j) Y_j' = \left(h\widehat{b}_0 f(t_0, y_0) + \sum_{j=1}^s (\widehat{d}_j - d_j) Z_j \right),$$

where $Z_j = Y_j - y_0$ and $d = b^{\top} A^{-1}$.

(a) Make clear: With adequate choice of \hat{d}_i the error $err := \hat{y}_1 - y_1$ fulfills

$$||err|| = Ch^{s+1} + O(h^{s+2}).$$

(b) Applying this error bound to the test equation $y' = \lambda y$, $y(0) = y_0$, for $h\lambda \to \infty$, the error bound behaves like $\hat{b}_0 h\lambda y_0$ (why?) and therefor is not useful for stiff differential equations. If one uses

$$err := (I - h\widehat{b}_0 J)^{-1}(\widehat{y}_1 - y_1),$$
 (1)

then $err \to -y_0$ for $h\lambda \to \infty$, where $J = \lambda I$ is the Jacobi matrix of the test equation. In the first and every rejected step (||err|| > 1) we set

$$\widehat{err} := (I - h\widehat{b}_0 J)^{-1} (h\widehat{b}_0 f(t_0, y_0 + err) + \sum_{j=1}^s (\widehat{d}_j - d_j) Z_j).$$

With this we get $\widehat{err} \to 0$ for $h\lambda \to \infty$ as for the numerical solution. Show these statements.

(c) How to regulate the step size? For the error (1) in the *n*th step, (so at time t_{n+1}) it holds $||err_{n+1}|| = C_n h_n^{s+1}$ (why?). Under the sometimes unrealistic assumption $C_{n+1} \approx C_n$ we obtain under an estimate for err_{n+1} and the request that $||err_{n+1}|| \approx 1$ the step size for the next step as

$$h_{new} := fac \cdot h_{old} \|err_{n+1}\|^{-1/(s+1)}$$
(2)

with the same weighted norm

$$||err_{n+1}|| = \sqrt{\frac{1}{d} \sum_{i=1}^{d} \left(\frac{err_{n+1,i}}{sc_i}\right)^2}, \quad sc_i = Atol_i + \max\{|y_{n,i}|, |y_{n+1,i}|\}Rtol_i.$$

and a factor fac which is dependent on the maximal number of Newton steps k_{max} and the number of made Newton iterations Newt in the current Runge Kutta step. It is given by

$$fac = 0.9 \cdot \frac{2k_{\text{max}} + 1}{2k_{\text{max}} + Newt}.$$

Here, $Atol_i$ and $Rtol_i$ are tolerances for the absolute and relative error.

In the case $h_{new} < fac \cdot h_{old}$ it follows $||err_{n+1}|| > 1$ (why?), i.e. a step size reduction of more than fac is not possible without rejection of the step.

(d) A realistic assumption is $C_{n+1}/C_n \approx C_n/C_{n-1}$. Show that from $C_{n+1}h_{new}^{s+1} = 1$ it follows for the new step size

$$h_{new} := fac \cdot h_n \left(\frac{1}{\|err_{n+1}\|} \right)^{1/(s+1)} \cdot \frac{h_n}{h_{n-1}} \left(\frac{\|err_n\|}{\|err_{n+1}\|} \right)^{1/(s+1)}. \tag{3}$$

A possible step size strategy lies for example in the choice of the minimum from (2) and (4).

Solutions are discussed on 19.06.2024.

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