Numerical Methods for Differential Equations exam **2015-12-18**
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Exam duration 14:00 – 18:00. A minimum of 16 points out of 32 are required to pass. Your grade is determined by the sum of your exam and project scores, in accordance with the rules published on the course home page.

No computers, pocket calculators, cell phones, browsing tablets or any other electronic devices, and no textbooks, lecture notes or written material, may be used during the exam.

1. **(5p)** You are familiar with the two-step BDF2 metod, i.e.

$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = hf(y_{n+1})$$

for the initial value problem

$$y' = f(y); \qquad y(0) = y_0.$$

The BDF2 method is implicit and and of order $p = 2$. One can also construct an implicit two-step method of order $p = 3$ using the same ρ polynomial as above, having the form

$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = h\beta_2 f(y_{n+1}) + h\beta_1 f(y_n) + h\beta_0 f(y_{n-1}).$$

(a) Determine the coefficients $\beta_0, \beta_1, \beta_2$ so that the consistency order is $p = 3$. (3p)

(b) Is the resulting method *zero-stable*? (Motivate your answer.) (1p)

(c) Is the resulting method *A-stable*? (Motivate your answer.) (1p)

Solution. We determine the order of consistency (and hence the coefficients) by verifying that the formula holds exactly for $y(t) = P(t) = t^m$ for $m = 0, 1, 2, 3$. We take the points $t_j = jh$ for $j = 0, 1, 2$. For $m = 0$ the left hand side (LHS) is 0, as is the right-hand side (RHS), and no conditions on the coefficients are obtained. For $m = 1$, the LHS is $3h - 2h + 0 = h$, while the RHS equals $h(\beta_2 + \beta_1 + \beta_0)$ giving the condition $\beta_2 + \beta_1 + \beta_0 = 1$. For $m = 2, 3$ we get

$$\frac{3}{2}(2h)^m - 2h^m + \frac{1}{2}0^m = h\beta_2 m(2h)^{m-1} + h\beta_1 m h^{m-1} + h\beta_0 0^{m-1}.$$

Hence, for consistency order $p = 3$, we have the linear system

$$\begin{aligned} \beta_2 + \beta_1 + \beta_0 &= 1 \\ 4\beta_2 + 2\beta_1 &= 4 \\ 12\beta_2 + 3\beta_1 &= 10 \end{aligned}$$

with solution $\beta_0 = -1/3$, $\beta_1 = 2/3$, $\beta_2 = 2/3$. The method is zero stable, because it shares its ρ polynomial with the BDF2 method,

$$\rho(w) = \frac{3}{2}(w-1)(w-\frac{1}{3}),$$

whose roots satisfy the root condition. The new method is not A-stable, though, because it is a third order method, and by the Dahlquist barrier theorem, the maximal order of an A-stable linear multistep method is $p = 2$. (This can also be easily verified in this case by applying the method to the linear test equation and showing that at least one root of the characteristic equation is outside the unit circle when $h\lambda$ is large and negative.

2. **(5p)** Consider the 3-stage embedded Runge-Kutta pair of orders $p = 2$ and $p = 3$ given by the Butcher tableau

0	0	0	0
1/2	1/2	0	0
3/4	0	3/4	0
M_1	0	1	0
M_2	2/9	3/9	4/9

where "M_1" refers to the first method and "M_2" to the second.

(a) Write the methods in terms of *stage values and stage derivatives*, when they are applied to the problem $\dot{y} = f(y)$. (1p)

(b) Determine the stability functions $R(h\lambda)$ for both methods. (2p)

(c) Which method is of order 2 and which is of order 3? (1p)

(d) Explain how an error estimate is obtained from "M_1" and "M_2" to make the method adaptive. (1p)

Solution. In terms of stage values and derivatives,

$$\begin{aligned} hY_1' &= hf(y_n) \\ hY_2' &= hf(y_n + hY_1'/2) \\ hY_3' &= hf(y_n + 3 \cdot hY_2'/4), \end{aligned}$$

with the first method advancing the solution by the 2nd order "modified Euler" method

$$y_{n+1} = y_n + hY_2', \tag{1}$$

and the second method according to

$$\hat{y}_{n+1} = y_n + \frac{1}{9}\left(2 \cdot hY_1' + 3 \cdot hY_2' + 4 \cdot hY_3'\right). \tag{2}$$

Hence the second method is the 3rd order method. An error estimate for controlling the step size is obtained from the difference $r_{n+1} = \|y_{n+1} - \hat{y}_{n+1}\|$. The stability polynomials are obtained by applying the methods to $\dot{y} = \lambda y$, using $y_n = 1$, from which we obtain

$$\begin{aligned} hY_1' &= h\lambda \\ hY_2' &= h\lambda(1 + h\lambda/2) = h\lambda + (h\lambda)^2/2 \\ hY_3' &= h\lambda(1 + 3 \cdot hY_2'/4) = h\lambda + 3(h\lambda)^2/4 + 3(h\lambda)^3/8, \end{aligned}$$

after which we obtain, for method 1,

$$y_{n+1} = 1 + h\lambda + \frac{(h\lambda)^2}{2}, \tag{3}$$

and for the second method,

$$\hat{y}_{n+1} = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{6}. \tag{4}$$

This confirms that it's the first method that is order 2, and the second method that is order 3.

3. **(5p)** The following nonlinear two-point boundary value problem is given:

$$\begin{aligned} &y'' + x(y^2)' - 2y^2 = g(x) \\ &y(0) = 1; \quad y'(1) = 1. \end{aligned}$$

   (a) Introduce a grid and discretize with a standard *second order* finite difference method. Be careful to define Δx, write down all equations, and show exactly how the boundary conditions affect the system by writing down the first and last equations separately. (4p)

   (b) As the resulting equation system is nonlinear, you will need to solve it by Newton's method. Construct the *last row* of the *Jacobian matrix* of the system of equations. (1p)

Solution. We introduce an equidistant grid with N internal points and $\Delta x = 1/(N+1/2)$, in order to treat the Neumann condition on the right. Here, $x_n = n \cdot \Delta x$. The discretization becomes

$$\frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta x^2} + x_n \frac{y_{n+1}^2 - y_{n-1}^2}{2\Delta x} - 2y_n^2 = g(x_n),$$

The left boundary condition is $y_0 = 1$ and the right Neumann condition is approximated by

$$y'(1) \approx \frac{y_{N+1} - y_N}{\Delta x} := 1,$$

which yields $y_{N+1} = \Delta x + y_N$. In all, the nonlinear system becomes

$$\begin{aligned}
\frac{-2y_1 + y_2}{\Delta x^2} + x_1 \frac{y_2^2}{2\Delta x} - 2y_1^2 &= g(x_1) - \frac{1}{\Delta x^2} + \frac{x_1}{2\Delta x} \\
\frac{y_{n-1} - 2y_n + y_{n+1}}{\Delta x^2} - x_n \frac{y_{n-1}^2 - y_{n+1}^2}{2\Delta x} - 2y_n^2 &= g(x_n) \\
\frac{y_{N-1} - y_N}{\Delta x^2} - x_N \frac{y_{N-1}^2 - (\Delta x + y_N)^2}{2\Delta x} - 2y_N^2 &= g(x_N) - \frac{1}{\Delta x}.
\end{aligned}$$

The last row of the Jacobian matrix therefore becomes

$$\left(0 \quad 0 \ldots 0 \quad \frac{1 - x_N y_{N-1} \Delta x}{\Delta x^2} \quad - 4y_N - \frac{1}{\Delta x^2} + x_N \frac{\Delta x + y_N}{\Delta x}\right)$$

4. **(5p)** Consider the following two-point boundary value problem:

$$\begin{aligned}
&y'' + Ky = -g(x) \\
&y(0) = 0, \qquad y(1) = 0,
\end{aligned}$$

where K is a real constant. The solvability of this problem depends on whether the problem is elliptic or not. This is governed by the properties of the operator

$$\mathcal{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + K,$$

which obviously depends on K.

(a) Use integration by parts to find the *logarithmic norm* $\mu_2[\mathcal{L}]$. (3p)

(b) Find out exactly for what values of K we have $\mu_2[\mathcal{L}] < 0$ and explain what happens if $K = \pi^2$. (2p)

Solution. Consider $\langle y, \mathcal{L}y\rangle = \langle y, y''\rangle + K\langle y, y\rangle$ and integrate by parts to get

$$-\langle y', y'\rangle + K\langle y, y\rangle \le (K - \pi^2)\langle y, y\rangle,$$

where the last inequality is due to Sobolev. So

$$\mu_2[\mathcal{L}] = K - \pi^2,$$

as equality holds for $y(x) = \sin \pi x$. Now $\mu_2[\mathcal{L}] < 0$, provided that $K < \pi^2$. That is, any negative K is fine, but K must not become large and positive. What happens if $K = \pi^2$? Then $\mathcal{L}$ has a zero eigenvalue and ellipticity is lost, in which case the solution is no longer unique. (For if $y(x)$ is a particular solution, solving $\mathcal{L}y = -g$, then $u(x) = y(x) + A \cdot \sin \pi x$ is also a solution to the system, since $\mathcal{L} \sin \pi x = 0$.)

5. **(5p)** Consider the following PDEs for $t \ge 0$ and $x, y \in [0, 1]$:

   (a) $u_t = \frac{1}{\mathrm{Pe}} u_{xx} + u_x$

   (b) $u_{tt} = u_{xx} + u_{yy}$

   (c) $u_{xx} + u_{yy} = f(x, y)$

   (d) $u_t + uu_x = 0$

   (e) $u_t = (d \cdot u_x)_x + f(u)$

   For each equation, classify the problem as *elliptic, parabolic or hyperbolic.* In addition, give the *name* of each equation, or, in case it has no name, name it based on the terms that enter the equation.

   Solution. The first is the parabolic *convection–diffusion equation*; the second is the hyperbolic *wave equation* in 2D; the third is the elliptic *Poisson equation* in 2D; the fourth is the hyperbolic *inviscid Burgers equation* (nonlinear conservation law); and the fifth is the parabolic *reaction-diffusion equation.*

6. **(7p)** Let the simple convection–diffusion equation, $u_t = u_{xx} + u_x$, with homogeneous Dirichlet conditions on $[0, 1]$, be discretized using the method of lines, to obtain a linear system of ODEs, $\dot{y} = (T_{\Delta x} + S_{\Delta x})y$.

   (a) What are the $N \times N$ matrices $T_{\Delta x}$ and $S_{\Delta x}$ when a second order discretization in space is used? (2p)

   (b) Explain why the method of lines ODE can be considered *stiff.* (1p)

(c) As stiff problems require implicit time-stepping, apply the trapezoidal rule to obtain a full discretization. Construct the system of equations that needs to be solved on each step and show, e.g. using the logarithmic norm or eigenvalue information, that the system has a *unique solution* for all $\Delta t > 0$. (2p)

(d) Given that

- $\lambda_k[T_{\Delta x} + S_{\Delta x}] = -2(N+1)^2 \left(1 - \sqrt{1 - \frac{\Delta x^2}{4}} \cos \frac{k\pi}{N+1}\right) < 0$;

  and

- $\lambda_k[R(A)] = R(\lambda_k[A])$ for every rational function R and every matrix A for which the expressions are defined;

show that the trapezoidal rule is *unconditionally stable* for this convection–diffusion equation (i.e., that there is no CFL restriction on the time step Δt). (2p)

Solution. The matrices are

$$T_{\Delta x} = \frac{1}{\Delta x^2} \text{tridiag}(1 \quad -2 \quad 1); \qquad S_{\Delta x} = \frac{1}{2\Delta x} \text{tridiag}(-1 \quad 0 \quad 1).$$

The problem is stiff because $T_{\Delta x} + S_{\Delta x}$ has large negative real eigenvalues, hence strong exponential damping. This is due to $T_{\Delta x}$, i.e., it is due to the presence of the diffusion term u_{xx} in the original equation. Because of the large negative eigenvalues, no matter what explicit time stepping method one would choose, there will be a CFL condition of the form $\Delta t / \Delta x^2 < C$, which is prohibitive; the time stepping method "stalls," and almost can't make any progress.

For a system $\dot{y} = Ay$, the trapezoidal rule is

$$y^{n+1} = y^n + \frac{\Delta t}{2}(Ay^n + Ay^{n+1}),$$

which means that one has to solve the linear system

$$(I - \frac{\Delta t}{2}A)y^{n+1} = (I + \frac{\Delta t}{2}A)y^n$$

on every step. Here $A = T_{\Delta x} + S_{\Delta x}$. Because we know that $\lambda_k[T_{\Delta x} + S_{\Delta x}] < 0$ it follows that

$$\lambda_k[I - \frac{\Delta t}{2}(T_{\Delta x} + S_{\Delta x})] = 1 - \frac{\Delta t}{2}\lambda_k[T_{\Delta x} + S_{\Delta x}] > 0$$

for all $\Delta t > 0$, so the matrix cannot be singular. Therefore there is a unique solution for all $\Delta t > 0$.

It also follows that there is no CFL condition: because the trapezoidal rule is A-stable, the product

$$\Delta t \lambda_k [T_{\Delta x} + S_{\Delta x}] < 0$$

for all $\Delta t > 0$, i.e., the eigenvalues always remain inside the stability region of the method. Thus there is no restriction on Δt.