CS 624: Numerical Solution of Differential Equations
Spring 2002
Problem Set 2

Handed out: Wed., Feb. 13.

Due: Fri., Feb. 22 in lecture.

1. Exercise 1.8.1 of the text. Restrict attention to consistent, D-stable explicit LMS formulas. [Hints: (1) First, argue that any D-stable consistent LMS has at least one nonzero β_j. This is established by arguing that $C_0 = 0 \Rightarrow \rho(1) = 0$, then D-stability $\Rightarrow \rho'(1) \neq 0$, then $\rho'(1) \neq 0, C_1 = 0 \Rightarrow$not all β_j's are zero. (2) If $p(z) = z^s + a_{s-1}z^{s-1} + \cdots + a_0$ is a monic polynomial, then for each i, a_{s-i} is the sum of all possible i-fold products of the roots, multiplied by a sign factor. In other words, if the roots of p are $z_1, \ldots, z_s$, then

$$a_{s-i} = (-1)^i \sum_{\{j_1,\ldots,j_i\}\subset\{1,\ldots,s\}} z_{j_1} \cdots z_{j_i}.]$$

2. In lecture it was argued that if all the real parts of A are negative in the linear constant-coefficient ODE $d\mathbf{u}/dt = A\mathbf{u}$, then $\mathbf{u}(t) \to \mathbf{0}$ as $t \to \infty$. Construct a 2×2 linear IVP $d\mathbf{u}/dt = A(t)\mathbf{u}$ (i.e., linear with nonconstant coefficients) such that all eigenvalues of $A(t)$ are negative real numbers bounded away from 0 for all t (i.e., all eigenvalues of $A(t)$ for all t are less than or equal to some constant $\lambda_{\max}$, and $\lambda_{\max} < 0$) yet $\mathbf{u} \to \infty$ as $t \to \infty$. Verify that your construction has an unbounded solution by computing trajectories with e.g. `ode45` in Matlab. (A proof of unboundedness is not required.)

   [Hint: first consider ODEs of the form $\mathbf{u}' = T\mathbf{u}$ where T is 2×2 upper triangular. Note that you can easily specify the eigenvalues of T. Find a T with negative eigenvalues and initial conditions such that the solution $\mathbf{u}$ blows up for awhile, and then dies off. Next consider $\mathbf{u}' = Q(t)TQ(t)^T\mathbf{u}$, where $Q(t)$ is 2×2 orthogonal. Figure out a way to define $Q(t)$ so that it moves mass from one entry of $\mathbf{u}$ to the other at exactly the right t-values to cause unbounded growth.]

3. Argue that if $A(t)$ is *real symmetric* and all the eigenvalues of $A(t)$ are negative for all t and bounded away from 0, then all solutions to $d\mathbf{u}/dt = A(t)\mathbf{u}$ tend to zero as $t \to \infty$. [Hint: consider $d(\mathbf{u}^T\mathbf{u})/dt$.]

4. Consider the reactions taking place in a homogeneous solution described by the chemical formulas $A + B \to C$ and $C \leftrightarrow D$, where A, B, C, D are compounds. There are three reactions here (namely $A + B \to C$, $C \to D$ and $C \leftarrow D$); let the three rate constants be m_1, m_2, m_3. Let $\alpha, \beta, \gamma, \delta$ be the concentrations of A, B, C, D as functions of t. Then the equations governing this system are

$$\alpha' = -m_1\alpha\beta,$$

$$\begin{aligned}
\beta' &= -m_1\alpha\beta, \\
\gamma' &= m_1\alpha\beta - m_2\gamma + m_3\delta, \\
\delta' &= m_2\gamma - m_3\delta.
\end{aligned}$$

Suppose the initial conditions are $a^0 = \beta^0 = 1$, $\gamma^0 = \delta^0 = 0$. Suppose the rate constants are $m_1 = 1$, $m_2 = 10000$, $m_3 = 1$. This means that A and B are slowly converted to C, C is very rapidly converted to D, and D is slowly converted back to C. So at the end of the reaction, one would expect most of the product to be D.

Integrate the above equations out to $t = 6$ in Matlab using `ode23` and `ode15s`. Note that `ode15s` is intended for stiff problems like this one. For `ode15s`, experiment with both numerical Jacobians (the default) and user-specified Jacobians. For user-specified Jacobians, you have to write code to provide the Jacobian. The help-files on these functions will explain how they work. Turn in plots of the concentrations of C and D for the various methods.

Hand in listings of all m-files, at least two interesting plots, and a couple of paragraphs describing your experience with these methods.