Elementary Numerical Analysis (409.310A)

Final Examination

12/12/05

1. Answer the following questions as concisely as possible. (15 points)
   1) Suppose that the eigenvalues of matrices A and B are {1.00, 0.99, 0.95, ..} and {1.10, 0.99, 0.91, ..}, respectively. The power method is applied to update the largest eigenvalue. If the same convergence is to be reached in both cases, how would the number of iterations for Matrix A be compared with that of Matrix B? Give only a rough estimate.
   2) How much error reduction would you expect if you halve the interval size in the integration using the Simpson rule? Give a short explanation to your answer.
   3) What is the difference between the explicit method and implicit method in solving an ordinary differential equation? Explain with the gain and cost of using an implicit method.
   4) Which matrix would rotate vector $(1,1,\sqrt{2})$ onto the x axis which would make the last two entries zero? Namely find the Householder transform matrix. You can just show the process, no need to find the exact final form of the matrix.

2. Consider the following one-dimensional eigenvalue problem involving particle diffusion. (20 points)

$$-\frac{d^2\phi}{dx^2}+\sigma\phi=\gamma\sigma_s\phi \qquad \text{where } \left.\frac{d\phi}{dx}\right|_{x=0}=0 \text{ and } \phi(L)=0$$

Note that diffusion coefficient is set to 1.0 and the reflective condition is given at the left boundary while the zero flux boundary condition is given at the right boundary ($x=L$). We would like to find the ***minimum*** eigenvalue γ and its corresponding vector. The coefficients defining the loss and production are assumed to be constant. Answer the following:

1) Discretize the equation by dividing the domain into 4 intervals and show that the resulting problem is a matrix eigenvalue problem which appears as:

$$A\phi=\gamma S\phi$$

$$A=\begin{bmatrix}1+h^2\sigma & -1 & & \\ -1 & 2+h^2\sigma & -1 & \\ & -1 & 2+h^2\sigma & -1 \\ & & -1 & 3+h^2\sigma\end{bmatrix},\ S=h^2\sigma_s\begin{bmatrix}1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1\end{bmatrix};\ \phi=\begin{bmatrix}\phi_1\\ \phi_2\\ \phi_3\\ \phi_4\end{bmatrix};\ h=\frac{L}{4}$$

Use the fact that you can introduce an imaginary node outside the boundary to reflect the boundary condition properly and the function value at the imaginary node is the same as the boundary function value with either the same sign or the opposite sign depending on the boundary condition.

2) Suppose that we are first interested in the ***maximum*** eigenvalue of matrix A before we find the minimum eigenvalue of the system. Apply the power method to find the first two iterates of the eigenvector and eigenvalue given the following conditions:

$$h^2\sigma=1$$
$$\phi^{(0)}=[1,0,0,0] \qquad \text{Hint : the resulting } \lambda^{(2)}=\frac{17}{5}$$
$$\lambda^{(0)}=1.0$$

3) Now, give an algorithm to find the ***minimum*** eigenvalue of the system.

4) The analytic solution for the n-th eigenfunction is obtained as $\phi_n(x)=\cos\frac{n\pi}{2L}x$. Derive the

dominance ratio of the system from the first and second eigenfunctions. Discuss the dependence of the dominance ratio on the domain size and the reaction coefficient σ.

3. Answer the following questions regarding the methods for finding various eigenvalues of a matrix. Give brief answers with only essential details. (15 Points)
   1) Explain and compare the deflation method and the decontamination method.
   2) What is the basic idea and procedure of the QR method? Explain then the need for the Householder transformation.

4. We would like to derive the Gaussian quadrature with 4 points. Noting that the points for which the function values are to be evaluated will be located symmetrically on the x axis between [-1,1] and the weights at the two symmetric points would be the same, we can set only two points in the positive half [0,1] and also two weighting factors as unknowns to determine, namely, $[x_1, x_2, w_1, w_2]$. Now answer the following: (15 points)
   1) What is the highest order of the polynomial that should give the exact integral when the 4 point Gaussian quadrature is used?
   2) Derive the 4 constraint equations to define the four unknowns. Note that the conditions for odd order polynomials is used already ~~to~~ by above reasoning to have only 4 unknowns.
   3) How would the two positions be related with the roots of a Legendre polynomial?
   4) Give the expression for w_1 in terms of the integration of the Lagrange polynomial?

5. Answer the following questions regarding finding the roots of nonlinear equations. (15 Points)
   1) Write an algorithm to implement the Newton-Raphson method. Consider explicitly the termination criteria.
   2) Suppose that there are many roots in the nonlinear equation of interest. How would you use the roots previously found to find another root?

6. Answer the following questions regarding the solution of ordinary differential equations. (20 Points)
   1) Show that the predictor-corrector scheme is third order accurate locally and then it is second order accurate globally.
   2) Give the fourth-order Runge-Kutta method to solve a coupled ODE $\frac{dy}{dt} = A(t)y + f(t)$ where y and f are vectors and A is a matrix.

7. Explain the two-parameter Chebyshev extrapolation method giving answers to the following questions. (Bonus Points)
   1) Suppose that you are at the k-th step in the iteration sequence and you want to use the most recent two estimates of the eigenvector and the one that you can obtain easily by the power method at the current step. Give an extrapolation expression using the three eigenvector estimates.
   2) Explain that this extrapolation scheme would increase the order of the polynomial to be used to represent the eigenvector estimate as a linear combination of all eigenvectors.
   3) Suppose that the resulting form of the new eigenvector estimate is given as the following

   $$x^{(k)} = c_1\eta_k(\gamma_1)u_1 + \sum_{i=2}^{n} c_i\eta_k(\gamma_i)u_i$$

   where $\eta_k(t)$ is a k-th order polynomial of t and $\gamma_i = \frac{2\lambda_i}{\lambda_2} - 1$. What is the rationale that $\eta_k(t)$ should be a constant multiple of the Chebyshev polynomial?
   4) How are the two extrapolation parameters determined? Explain briefly with only words.