Qualifying Examination in Numerical Analysis (580-780), August 2008

Direction: There are three categories of problems. Select one and only one problem from each category and answer all the subproblems. Use only one side of the paper to write your answers. Clearly identify the problem and all subproblem numbers on your answer sheets.

Category A

A1. Given a symmetric matrix $A \in \mathbb{R}^{n\times n}$, define its associated Rayleigh quotient $\rho(\mathbf{x})$ for any nonzero $\mathbf{x} \in \mathbb{R}^n$ by the scalar-valued function

$$\rho(\mathbf{x}) := \frac{\mathbf{x}^\top A\mathbf{x}}{\mathbf{x}^\top \mathbf{x}}. \tag{1}$$

1. Suppose that the eigenvalues of A are arranged in the order

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

   (a) Show that for all nonzero $\mathbf{x} \in \mathbb{R}^n$, it is true that

$$\lambda_1 \geq \rho(\mathbf{x}) \geq \lambda_n.$$

   (b) Show that the two extreme values of $\rho(\mathbf{x})$ are attainable by some $\mathbf{x}$. Specify these optimizers.

2. Let $\mathbf{y} \in \mathbb{R}^n$ be an arbitrary vector. Show that the smallest eigenvalue of $A + \mathbf{y}\mathbf{y}^\top$ is greater than or equal to the smallest eigenvalue of A.

3. One way to find an eigenvalue/eigenvector pair $(\lambda, \mathbf{x})$ of the matrix A is to solve the system of $n+1$ nonlinear equations

$$F(\boldsymbol{\phi}) = \begin{pmatrix} A\mathbf{x} - \lambda\mathbf{x} \\ \mathbf{c}^\top\mathbf{x} - 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{2}$$

   where $\mathbf{c} \in \mathbb{R}^n$ is a fixed constant vector, for the unknown vector $\boldsymbol{\phi} = (\lambda, \mathbf{x}^\top) \in \mathbb{R}^{n+1}$.

   (a) What is the Jacobian of this system?

   (b) What are the equations for $\boldsymbol{\phi}_{k+1}$ in a Newton step?

   (c) Make an argument that the Newton method is equivalent to an inverse power method with shift λ_k.

4. In the shifted inverse power method

$$(A - cI)\mathbf{z}_{k+1} = \mathbf{z}_k, \tag{3}$$

   the closer the shift c is to an eigenvalue, the more ill-conditioned is the matrix $A - cI$. Consequently, the computed $\mathbf{z}_{k+1}$ typically would be far from being accurate. How can such an inaccurate computation still be useful for eigenvalue computation?

A2. Suppose $\overline{\mathbf{x}}$ has been computed in solving the linear system $A\mathbf{x} = \mathbf{b}$, where A is a nonsingular square matrix. Let $\mathbf{r} := \mathbf{b} - A\overline{\mathbf{x}}$ be the residual.

1. Show that

$$\frac{\|\mathbf{x} - \overline{\mathbf{x}}\|_p}{\|\mathbf{x}\|_p} \leq \kappa_p(A)\frac{\|\mathbf{r}\|_p}{\|\mathbf{b}\|_p}, \tag{4}$$

   where $\kappa_p(A) = \|A\|_p\, \|A^{-1}\|_p$ and $\|\cdot\|_p$ denotes the p-norm.

2. Show that if $A = QR$ is the QR decomposition of A, then $\kappa_2(A) = \kappa_2(R)$ and

$$\frac{1}{n}\kappa_1(A) \leq \kappa_1(R) \leq n\kappa_1(A). \tag{5}$$

3. The difficulty associated with the condition number is the computation of $\|A^{-1}\|$, which requires $O(n^3)$ flops. One idea is to choose a vector $\mathbf{d}$ and solve the systems

$$R^\top \mathbf{z} = \mathbf{d}, \quad R\mathbf{y} = \mathbf{z}. \tag{6}$$

   (a) Show that $\gamma_p(\mathbf{d}) := \|\mathbf{y}\|_p/\|\mathbf{z}\|_p \leq \|A^{-1}\|_p$.

   (b) What is the cost of these estimate in terms of n? Justify your answer.

4. Suppose $A = U\Sigma V^\top$ is the singular value decomposition of A with singular values

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n.$$

   (a) What is $\|A^{-1}\|_2$ in terms of the singular values of A?

   (b) Expand the vector $\mathbf{d}$ in (6) in terms of the columns $\{\mathbf{v}_i\}$ of V, that is, $\mathbf{d} = \sum_{i=1}^n d_i \mathbf{v}_i$. Show that

$$\gamma_2(\mathbf{d}) = \left(\frac{\sum_{i=1}^n (d_i/\sigma_i^2)^2}{\sum_{i=1}^n (d_i/\sigma_i)^2} \right)^{1/2}. \tag{7}$$

   (c) Under what conditions is $\gamma_2(\mathbf{d})$ a good estimate to $\|A^{-1}\|_2$?

Category B

B1. This question concerns various forms and properties of quadratures.

1. Let $C[a,b]$ denote the set of all continuous functions $f : [a,b] \to \mathbb{R}$. The space $C[a,b]$ is equipped with a natural norm

$$\|f\| := \max_{x \in [a,b]} |f(x)|.$$

   For any *linear functional* $\mathcal{F} : C[a,b] \to \mathbb{R}$, define the dual norm of $\mathcal{F}$ by

$$\|\mathcal{F}\| := \sup_{\|f\|=1} |\mathcal{F}(f)|. \tag{8}$$

   (a) Compute the dual norm of the functional $\mathcal{F}(f) = \int_a^b f(x)dx$ for $f \in c[a,b]$.

   (b) Suppose the integral $\mathcal{F}$ is replaced by a quadrature $\mathcal{Q}$. Show that if

$$\mathcal{Q}(f) \quad := \quad \sum_{i=1}^n a_i f(t_i), \tag{9}$$

   where t_i, $i = 1, \ldots, n$, are some fixed points in $[a,b]$, then

$$\|\mathcal{Q}\| \quad = \quad \sum_{i=1}^n |a_i|. \tag{10}$$

2. Derive an integration formula of the form

$$\int_0^h f(\sqrt{x})dx \approx \omega_1 f(0) + \omega_2 f(h/2) + w_3 f(h) \tag{11}$$

   which is exact for quadratic polynomials.

3. With respect to a weight function $\omega(x) \geq 0$ over the interval $[-1,1]$, define the inner product of two functions by

$$\langle f, g \rangle = \int_{-1}^1 f(x)g(x)\omega(x)dx \tag{12}$$

and the norm $|||f||| = \langle f, f\rangle^{1/2}$, whenever the integrals exist. With respect to this inner product, a sequence of orthogonal polynomials $\{p_k(x)\}$, $k = 0, 1, \ldots$, can be defined, that is, $p_k(x)$ is a polynomial of degree precisely k and satisfies $\langle p_k, p_m\rangle = 0$ if $m \neq k$. For any function $f \in C[-1, 1]$ and for any positive integer n, define the polynomial

$$\mathcal{L}_n(f)(x) = \sum_{k=0}^{n} \hat{f}_k p_k(x), \tag{13}$$

with coefficients

$$\hat{f}_k = \frac{\langle f, p_k\rangle}{\langle p_k, p_k\rangle}. \tag{14}$$

Show that $\mathcal{L}_n(f)$ is the best least squares polynomial approximation to f in the sense that it minimizes $|||f - q|||$ among all polynomials $q(x)$ of degree less than or equal to n.

4. Derive a least squares integration formula for the integral $\int_{-3h}^{3h} f(x)dx$ by first making a least squares approximation to $f(x)$ by a quadratic polynomial $q(x)$ at the five points $-3h$, $-2h$, 0, $2h$, and $3h$; and then integrating $q(x)$.
   (a) Show that the least squares quadrature is of the form

$$\int_{-3h}^{3h} f(x)dx \approx a_1 f(-3h) + a_2 f(-2h) + a_3 f(0) + a_4 f(2h) + a_5 f(3h). \tag{15}$$

   (b) Describe a method to compute the five coefficients a_i, $i = 1, \ldots, 5$.

B2. This question concerns numerical ODE methods.

1. The initial value problem

$$y' = \sqrt{y}, \quad y(0) = 0 \tag{16}$$

has the nontrivial solution $y(x) = (x/2)^2$. Application of the forward Euler method with any step size h however yields $y_n \equiv 0$ for all n. Explain this paradox.

2. Suppose the method

$$y_{n+2} + 9y_{n+1} - 10y_n = \frac{h}{2}(13f_{n+1} + 9f_n) \tag{17}$$

is applied to the initial value problem

$$y' = 0, \quad y(0) = c. \tag{18}$$

Let the starting values be $y_0 = c$ and $y_1 = c + \epsilon$, where ϵ is the machine precision. What values y_n are to be expected for arbitrary step size h?

3. Assume that a vector-valued function $\mathbf{u}(x) = [u_1(x), \ldots u_{2n-1}(x)]^\top \in \mathbb{R}^{2n-1}$ is governed by the continous-time finite Lokta-Volterra differential equation

$$u_k' = u_k(u_{k+1} - u_{k-1}), \quad k = 1, \ldots, 2n-1, \tag{19}$$

where $u_0(x) = u_{2n}(x) \equiv 0$ for all x. The problem can be solved analytically as follows:
   (a) Make a change of variable via

$$u_k = \frac{\tau_{k+2}\tau_{k-1}}{\tau_{k+1}\tau_k}. \tag{20}$$

   Show that a compatible equation is

$$\frac{d\tau_k}{dt}\tau_{k+1} - \tau_k\frac{d\tau_{k+1}}{dt} + \tau_{k-1}\tau_{k+2} = 0. \tag{21}$$

   (*Hint: take natural logarithm on both sides.*)

(b) Starting with $\tau_{-1} \equiv 0$, $\tau_0 \equiv 1$, $\tau_1(t) = 1$ and $\tau_2(t) = \psi(t)$, show that

$$\begin{aligned} \tau_3 &= \frac{d\psi}{dt}, \\ \tau_4 &= \det \begin{bmatrix} \psi & \psi^{(1)} \\ \psi^{(1)} & \psi^{(2)} \end{bmatrix}, \end{aligned}$$

and so on.

4. A particular Euler-type discretization for (19) is given by

$$u_k^{[\ell+1]} = u_k^{[\ell]} + h\left(u_k^{[\ell]} u_{k+1}^{[\ell]} - u_k^{[\ell+1]} u_{k-1}^{[\ell+1]}\right). \tag{22}$$

where, not to be confused with the subscript k for the kth entry in $\mathbf{u}$, the superscript ℓ stands for the advance in time, i.e., $u_k^{[\ell]} \approx u_k(\ell h)$. Starting with a prescribed initial value $[u_1^{[0]}, \ldots, u_{2n-1}^{[0]}]^\top$, together with boundary conditions $u_0^{[\ell]} \equiv 0$ and $u_{2n}^{[\ell]} \equiv 0$ for all ℓ, sketch a mechanism or flowchart showing that the scheme (22) is actually an explicit method.

Category C

C1. Given a smooth function $f : \mathbb{R} \to \mathbb{R}$, consider the problem of finding its root $f(x^*) = 0$. Most numerical methods are iterative in nature.

1. A method based on a *linear model* takes two points a_k and b_k, interpolate $f(x)$ by a straight line there, then use the zero of this model as the next iterate. The iterative scheme for this approach is

$$x_{k+1} = x_k - \frac{f(a_k)}{f[a_k, b_k]}, \tag{23}$$

where $f[a,b] := \frac{f(b)-f(a)}{b-a}$ denotes the Newton's divide difference. Define the error $e_k := x^* - x_k$. Show that the error of an iterate from a linear model is

$$e_{k+1} = \frac{f[a_k, b_k, x^*]}{f[a_k, b_k]}(x^* - a_k)(x^* - b_k). \tag{24}$$

2. Suppose $f'(x^*) \neq 0$. Make an argument that the classical Newton method

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)},$$

is a special case of (23), provided a_k and b_k are sufficiently close to x^*. Deduce from (24) that the Newton's iterative method has an error

$$e_{k+1} = -\frac{f''(\xi_1)}{2f'(\xi_2)} e_k^2, \tag{25}$$

where ξ_1 and ξ_2 are points near x^* depending on k.

3. A method based on a *quadratic model* takes three points a_k, b_k, and c_k, interpolate $f(x)$ by a parabola there, then use the zero of this model as the next iterate. Sketch a prototype program that implements this idea for finding x^*.

4. Show that the error from the quadratic model is given by

$$e_{k+1} = -\frac{f[a_k, b_k, c_k, x^*]}{f[a_k, b_k] + f[a_k, b_k, c_k](2\xi - a_k - b_k)}(x^* - a_k)(x^* - b_k)(x^* - c_k), \tag{26}$$

where ξ is between x^* and x_{k+1}. (*Hint: use the Newton's divided difference interpolation formula.*)

C2. This question concerns the Krylov subspace methods.

1. Define the GMRES and CG iterations in terms of what problems they solve and what their iterations minimize.
2. Give a formula for the first GMRES iteration for $A\mathbf{x} = \mathbf{b}$ if the initial iterate is $\mathbf{x}_0 = 0$.
3. Let $\mathbf{y} \in \mathbb{R}^n$. Assume that $\|\mathbf{y}\| = 1$.
   (a) What are the eigenvalues of $I + \mathbf{y}\mathbf{y}^\top$?
   (b) Show that it takes at most two GMRES iterations to solve $(I + \mathbf{y}\mathbf{y}^\top)\mathbf{x} = \mathbf{b}$.
   (c) Is $I + \mathbf{y}\mathbf{y}^\top$ symmetric? Would symmetry help with your answer to question (b) above and GMRES in general?
   (d) Let E be an $n \times n$ matrix with $\|E\| \leq 10^{-1}$. Let

   $$A = I + \mathbf{y}\mathbf{y}^\top + E.$$

   How many GMRES iterations does it take to reduce the residual by a factor of 10^{-2}. (*Warning! You can't assume that A is diagonalizable. Hint: what is $(I - A)(2I - A)$?*)