PhD Qualifying Exam

Scientific Computing
November 25, 2010

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1. Consider $A = \begin{pmatrix} 0 & 1 & 2 \\ 2 & 0 & 0 \\ 0 & 1 & -2 \end{pmatrix}$.

   (a) Compute the *singular value decomposition* (SVD) of A.

   (b) Write down a best (2-norm) rank-one approximation X_1 of A, and specify $\|A - X_1\|_2$.

   (c) Consider the rank-one matrix $X = \sigma_3 u_1 v_1^*$ according to part SVD of A. What is $\|A - X\|_2$?

   (d) Describe infinitely many rank-one matrices X for which $\|A - X\|_2 = \|A - X_1\|_2$.

2. Consider evaluating the integral $\int_{-1}^{1} f(x)\,dx$.

   (a) Compute A and B so that the quadrature rule

   $$\int_{-1}^{1} f(x)\,dx \approx Af(0) + Bf'(0)$$

   is exact for *linear* polynomials.

   (b) Improve the quadrature rule by

   $$\int_{-1}^{1} f(x)\,dx \approx Af(0) + Bf'(0) + Cf''(0)$$

   so that it is exact for *quadratic* polynomials.

   (c) Is the Simpson's rule exact for cubic polynomials? Is it true for the method in part (b), above? If so, which one would you prefer, and why? Explain, and write down the Simpson's rule as well.

   (d) Assuming f to be sufficiently smooth, use Taylor expansion (with remainder) to derive a bound for

   $$\left| \int_{-1}^{1} f(x)\,dx - Af(0) + Bf'(0) + Cf''(0). \right|$$

3. Let $f \in C^3$, and $f'(x) > 0$ for any $x \in \mathbb{R}$. In order to find a zero of f, one can use the equivalent equation,

$$\frac{f(x)}{\sqrt{f'(x)}} = 0. \qquad (\star)$$

(a) Formulate the Newton's method (iterations) for $(\star)$. And apply two iterations of the formulation by choosing $f(x) = x^3$ and $x_0 = 1$ to compute x_1 and x_2.

(b) Prove its cubic convergence to a zero of f.

4. Let

$$(I + A)x = b, \tag{$\star$}$$

with $b \in \mathbb{R}^n$, $A = \frac{1}{4}(P_1 + P_2 + P_3)$, where $P_i \in \mathbb{R}^{n\times n}, i = 1, 2, 3$, are arbitrary permutation matrices.

(a) What is a permutation matrix?

(b) Show that $\|Px\|_2 = \|x\|_2$ for any permutation matrix $P \in \mathbb{R}^{n\times n}$, $x \in \mathbb{R}^n$.

(c) Show that $I + A$ is nonsingular, and give upper bounds for $\|A\|_2$, $\|I + A\|_2$, $\left\|(I + A)^{-1}\right\|_2$, and $\mathrm{cond}_2(I + A)$.
Hint: You may use the property that, if $X \in \mathbb{R}^{n\times n}$, $\|X\| < 1$ then $\left\|(I + A)^{-1}\right\| \leq \frac{1}{1-\|X\|}$.

(d) Show that the fixed point iteration

$$x^{(k+1)} = b - Ax^{(k)}, \quad k = 0, 1, \ldots \tag{$\star\star$}$$

is consistent with ($\star$).

(e) Show that the iteration ($\star\star$) converges linearly (with respect to the 2-norm), and give an estimate for its rate.

(f) Let the initial guess be $x^{(0)} = b$. Estimate the minimum number N of steps of ($\star\star$) required so that

$$\frac{\left\|x^{(N)} - x^\star\right\|_2}{\|x^\star\|_2} \leq 10^{-2}, \tag{RE}$$

where $x^\star$ is the solution of ($\star$).

(g) Formulate a (*a posteriori*) termination criterion that guarantees the inequality (RE) for any b as well as any initial guess $x^{(0)}$.

5. Let $f(x) = \sqrt{x}$ on $x \in [0, 1]$. Find the line that best approximates f in the least-squares (L^2-norm) sense. Also, find the associated error.

6. Let the data be given as $\{(0,\alpha),(1,1),(2,2),(3,0)\}$ for (t,y) pairs, where $\alpha \in \mathbb{R}$.

   (a) Compute a quadratic least-squares approximation

   $$p(t) = x_0 + x_1 t + x_2 t^2$$

   to the data.

   (b) Is there a value of α for which the polynomial p interpolates the data? If yes, is such an α unique?

7. Consider the eigenvalue problem

$$u''(x) = \lambda u(x), \qquad u(0) = u(\pi) = 0.$$

(a) Find all eigenvalues of λ for which a nonzero solution $u(x)$ exists.

(b) Use *centered* finite difference approximation to $u''(x)$ to convert the problem into a finite-dimensional eigenvalue problem

$$A\vec{u} = \lambda\vec{u}, \tag{$\star$}$$

where $\vec{u} = (u_1, \ldots, u_N)^\top$, $A \in \mathbb{R}^{N\times N}$, by discretising the interval $[0, \pi]$ as

$$x_j = jh, \quad h = \frac{\pi}{N+1}, \quad u_j \approx u(x_j)$$

for $j = 0, 1, \ldots, N+1$. Write down the matrix A.

(c) Use $N = 2$ to solve ($\star$). Compare your result with part (a) by drawing a picture to illustrate the solutions $u(x)$ and $\vec{u}$.

8. Let $x = [2,\ 3/2]^\top$.

(a) Compute a vector v such that the Householder reflector $H(v)$ yields

$$H(v)x = \begin{bmatrix} \|x\|_2 \\ 0 \end{bmatrix}.$$

(b) Compute $H(v)^* H(v)$ for this particular v to verify that $H(v)$ is unitary.

(c) Construct the orthogonal projector P onto $\operatorname{span}\{v\}$.

(d) Sketch, in two dimension, a rough (but clean) drawing that shows $\operatorname{span}\{v\}$, $\operatorname{span}\{v\}^\perp$, x, Px, $(I - P)x$, and $H(v)x$. Ensure that you label your illustration clearly.

(e) Find also the Givens rotation G, if it exists, so that $Gx = H(v)x$.