Fall 2014 Scientific Computation Comprehensive Exam

Answer **5 questions** *of your choice explaining all steps that lead to a solution. Partial credit will be awarded for presenting a viable solution strategy. No credit will be given to computations presented without explanation of the adopted approach.*

1. Find the quadratic polynomial which is the best approximation to $f(x) = x^3$ in $L_2[-1, 1]$.

2. For a given smooth function $f \in C^\infty[0, 1]$, let $h = 1/n$ and consider the composite midpoint rule

$$I(f) = \int_0^1 f(x)dx \approx h \sum_{i=1}^{n} f((i - 1/2)h) \equiv Q(f, n).$$

a) Prove that

$$I(f) = Q(f, n) + \frac{1}{24} Q(f'', n)h^2 + \frac{1}{1920} Q(f^{(4)}, n)h^4 + O(h^6),$$

$$I(f'') = Q(f'', n) + \frac{1}{24} Q(f^{(4)}, n)h^2 + O(h^4),$$

and

$$I(f^{(4)}) = Q(f^{(4)}, n) + O(h^2).$$

b) Prove that

$$I(f) - Q(f, n) = a_1 h^2 + a_2 h^4 + O(h^6).$$

Find explicit formulas for a_1 and a_2.

c) Assume that $f(x)$ is also periodic with fundamental period 1, discuss the convergence of the composite midpoint rule.

3. Consider the initial value problem

$$y'(t) = f(t, y), \quad y(0) = a,$$

and the linear multistep method with constant step size h

$$y_{n+2} + 4y_{n+1} - 5y_n = h(4f_{n+1} + 2f_n),$$

where $t_n = n * h$ and $f_n = f(t_n, y_n)$.

a) Assume $y_n = y(t_n)$ and $y_{n+1} = y(t_{n+1})$, show that

$$|y_{n+2} - y(t_{n+2})| \leq Ch^4,$$

for some constant $C > 0$ independent of h, provided that $f(t, y)$ is sufficiently smooth.

b) Given the initial data $y_0 = a$ and $y_1 = a + f(0, a)h$, show that for general smooth functions $f(t, y)$, the linear multistep method may generate poor approximation to the analytical solution. Explain why.

4. By analogy to the polar form of a complex scalar $z = e^{i\theta}\rho \in \mathbb{C}$, consider the polar decomposition of $A \in \mathbb{C}^{m\times n}$, $m \geqslant n$, as $A = UP$, with $U \in \mathbb{C}^{m\times n}$ a matrix with orthonormal columns, and $P \in \mathbb{C}^{n\times n}$ a positive semidefinite Hermitian matrix.

a) Prove that the polar decomposition exists, and is unique if A is nonsingular.

b) Use the polar decomposition to solve the least squares problem

$$\min_x \|Ax - b\|_2,$$

$x \in \mathbb{C}^n$, $b \in \mathbb{C}^m$.

5. The Lanczos algorithm results from incomplete reduction of $A \in \mathbb{R}^{m\times m}$, A symmetric, to tridiagonal form

$$A = QTQ^T,$$

with Q orthogonal, T tridiagonal. Following the same approach, write the unsymmetric Lanczos algorithm resulting from the factorization of $B \in \mathbb{R}^{m\times m}$

$$B = PTQ^T,$$

P, Q orthogonal, T tridiagonal.

6. Consider the differential equation problem

$$\begin{cases} u'' + \alpha u^2 & = & \sin \pi x \\ u(x=0) & = & 0 \\ u(x=1) & = & 0. \end{cases}$$

a) Using a uniform mesh of size h and the centered difference scheme, derive the discretized nonlinear algebraic system for the discrete solution $\mathbf{u} = [\mathbf{u}_1 \ldots \mathbf{u}_N]$ of the form

$$AU + F(U) = 0.$$

Identify A, F, and each equation explicitly.

b) Describe the details of how Newton's method can be used to solving this nonlinear system. Discuss the algorithm's efficiency.

c) Assume that a solution exists for all values of α. Write a numerical algorithm to compute α that maximizes $u(x = \frac{1}{2})$.

Aug 2014

Problem 1

Want to minimize: $E = \int_{-1}^{1} (x^3 - p(x))^2 \, dx$ where $p(x) = ax^2 + bx + c$

$$\Rightarrow \quad E = \int_{-1}^{1} (x^3 - ax^2 - bx - c)^2 \, dx$$

$$= \int_{-1}^{1} (x^6 - ax^5 - bx^4 - cx^3 - ax^5 + a^2x^4 + abx^3 + acx^2$$

$$-bx^4 + abx^3 + b^2x^2 + bcx - cx^3 + acx^2 + bcx + c^2) \, dx$$

(Integrating odd funcs on $[-1,1]$ will be zero so...)

$$= \int_{-1}^{1} (x^6 + (-b + a^2 - b)x^4 + (ac + b^2 + ac)x^2 + c^2) \, dx$$

$$= \frac{1}{7}x^7 + \frac{1}{5}(a^2 - 2b)x^5 + \frac{1}{3}(2ac + b^2)x^3 + c^2 x \Big]_{-1}^{1}$$

$$= 2/7 + \frac{2}{5}(a^2 - 2b) + \frac{2}{3}(2ac + b^2) + c^2$$

$$\frac{\partial E}{\partial a} = \frac{4}{5}a + \frac{4}{3}c = 0$$

$$\frac{\partial E}{\partial b} = -4/5 + \frac{4}{3}b = 0 \quad \Rightarrow \quad \begin{cases} 3a + 5c = 0 \\ b = 3/5 \\ 2a + 3c = 0 \end{cases} \quad \Rightarrow \quad a = c = 0$$

$$\frac{\partial E}{\partial c} = \frac{4}{3}a + 2c = 0$$

$\therefore$ The quadratic that minimizes E is: $\boxed{p(x) = \frac{3}{5}x}$

Problem 1

Aug 2014

Want to minimize: $E = \int_{-1}^{1} (x^3 - p_2(x))^2 \, dx$ ← $w(x)$

Alternate Soln

choose innerproduct: $\langle p, q \rangle = \int_{-1}^{1} p\, q \, dx$ ← $w(x)$

Gramm-Schmidt: $\{1, x, x^2\}$

$$u_0 = 1$$

$$u_1 = x - \frac{\langle 1, x \rangle}{\langle 1, 1 \rangle} \cdot 1 = x$$

$$u_2 = x^2 - \frac{\langle x^2, 1 \rangle}{\langle 1, 1 \rangle} \cdot 1 - \frac{\langle x^2, x \rangle}{\langle x, x \rangle} x = x^2 - 1/3$$

$$\int_{-1}^{1} f(x) u_k(x) \, dx = a_k \int_{-1}^{1} u_k^2(x) \, dx$$

(Get this from review notes

$k=0$: $\int_{-1}^{1} x^3 dx = a_0 \int_{-1}^{1} dx$

$$0 = a_0 (1+1)$$

$$a_0 = 0$$

$k=1$: $\int_{-1}^{1} x^3 x \, dx = a_1 \int_{-1}^{1} x^2 \, dx$

$$\int_{-1}^{1} x^4 \, dx = a_1 (2/3)$$

$$2/5 = a_1 (2/3)$$

$$a_1 = 3/5$$

$k=2$: $\int_{-1}^{1} x^3 (x^2 - 1/3) \, dx = a_2 \int_{-1}^{1} (x^2 - 1/3)^2 \, dx$

$$0 = a_2 \cdot \#$$

$$a_2 = 0$$

$$\boxed{p_2(x) = \frac{3}{5} x}$$

Problem 3 Aug 2014

$$\begin{cases} y'(t) = f(t,y) \\ y(0) = a \end{cases}$$

$$y_{n+2} + 4y_{n+1} - 5y_n = h(4f_{n+1} + 2f_n)$$

a) $y(t_n + 2h) = y(t_{n+2}) \approx y_{n+2} = -4y_{n-1} + 5y_n + h(4f_{n+1} + 2f_n)$

$$\Rightarrow y_n + 2hy' + 2h^2y'' + \frac{4h^3}{3}y''' + \frac{2h^4}{3}y^{(4)} \approx -4\left(y_n + hy_n' + \frac{h^2}{2}y'' + \frac{h^3}{3!}y''' + \frac{h^4}{4!}y^{(4)}\right)$$

$$+ 5y_n$$

$$+ 4h\left(y_n' + hy_n'' + \frac{h^2}{2}y''' + \frac{h^3}{3!}y^{(4)}\right)$$

$$+ 2hy_n$$

$\Theta(1)$: $1 = -4 + 5$ ✓

$\Theta(h)$: $2 = -4 + 4 + 2$ ✓

$\Theta(h^2)$: $2 = -2 + 4$ ✓

$\Theta(h^3)$: $4/3 = -\frac{2}{3} + 2$ ✓

$\Theta(h^4)$: $2/3 = -1/6 + \frac{2}{3}$

By defn of $\Theta(h^4)$ $\exists C$ st $|y(t_{n+2}) - y_{n+2}| < Ch^4$

b) We start by checking if our method is zero stable:

* Assume $y' = 0$ and $y_n = r^n$ $\Rightarrow$ $r^2 + 4r - 5 = 0$

$(r+5)(r-1) = 0$

$r = -5, 1$

$\Rightarrow y_n = c_1(-5)^{-n} + c_2(1)^n = c_1(-5)^n + c_2$

$\Rightarrow y_0 = c_1 + c_2 = a$ (b/c $y_0 = a$)

$y_1 = -5c_1 + c_2 = a + f(0,a)h = a + y_0' \underset{\uparrow \text{ by } *}{=} a$

$\begin{cases} c_1 + c_2 = a \\ -5c_1 + c_2 = a \end{cases} \Rightarrow c_1 = 0,\ c_2 = a \Rightarrow y_n = a$ (Makes sense $\because$ $y(x) = a$ is a soln in this case!)

But what if $y_0 = a + \varepsilon$?

$\Rightarrow \begin{cases} y_0 = c_1 + c_2 = a + \varepsilon \\ y_1 = -5c_1 + c_2 = a \end{cases} \Rightarrow c_1 = \varepsilon/6 \Rightarrow c_2 = a + \frac{5\varepsilon}{6}$

$\Rightarrow y_n = \frac{\varepsilon}{6}(-5)^n + a + 5\varepsilon/6$

$\Rightarrow |y_n - y(x)| = \left| \varepsilon/6\,(-5)^n + \frac{5\varepsilon}{6} \right| \longrightarrow \infty$ as $n \to \infty$

So it's not zero stable

Problem 4

Idea: $e^{i\theta} \to U \quad \rho \to P$

Note that $\rho \geq 0$ and $\rho = \sqrt{z^* z}$. So we can try to define P in the following ways:

$$\underset{n\times n}{P = \sqrt{A^* A}} \quad \text{or} \quad \cancel{\underset{m\times m}{P = \sqrt{AA^*}}}$$

↑ wrong dimensions

So we start by defining: $B = A^* A$

$\Rightarrow B$ is normal $\Rightarrow B$ is positive and semi-definite

Thus we can define B by the following:

$$B = X \Lambda X^* \qquad \lambda_{ii} \geq 0$$

$$= X C^2 X^*$$

$$= \underbrace{X C X^*}_{P} X C X^*$$

$$= P^2$$

$\Rightarrow P^2 = B$ Thus we have found P and n+f U.

Let v_i be an eigenvector of P and λ_i be the eigenvals.

$\Rightarrow A v_i = U P v_i = U \lambda_i v_i$

$\Rightarrow U v_i = \frac{1}{\lambda_i} A v_i$ for $\lambda_i > 0$.

If $\lambda_i = 0 \Rightarrow A v_i = 0 \Rightarrow$ we don't need anything from U

$$\Rightarrow U = [\underbrace{\tfrac{1}{\lambda_1} A v_1 \mid \tfrac{1}{\lambda_2} A v_2 \mid \dots \mid \tfrac{1}{\lambda_\ell} A v_\ell}_{\tilde{A}} \mid \phi_{\ell+1} \mid \dots \mid \phi_m] D$$

where $\lambda_i = \begin{cases} 0 & j > \ell \\ \neq 0 & j \leq \ell \end{cases}$ for som D and $\{\phi_\ell\}$ orthonormal

$\Rightarrow \quad \mathcal{U} v_i = \tilde{A} D v_i$

Need $D v_i$ to pick a colum of $\tilde{A}$ so: $\quad D = \begin{bmatrix} v_1^* \\ \hline v_2^* \\ \hline \vdots \\ \hline v_n^* \end{bmatrix}$

$\Rightarrow D v_i = e_i$

Q) Is $\{ \frac{1}{\lambda_i} A v_i \}$ orthonormal?

A) $\langle \frac{1}{\lambda_i} A v_i , \frac{1}{\lambda_i} A v_i \rangle = \langle \frac{1}{\lambda_i} v_i , A^* \frac{1}{\lambda_i} A v_i \rangle$

$= \langle \frac{1}{\lambda_i} v_i , \frac{1}{\lambda_i} P^2 v_i \rangle$

$= \langle \frac{1}{\lambda_i} v_i , \lambda_i v_i \rangle = \frac{\lambda_i}{\lambda_i} \delta_i = \delta_i$

$\Rightarrow \mathcal{U}$ exists and has the defined form.

Next sps A is non-singular

$\Rightarrow 0 \neq \det(A) = \det(\mathcal{U}) \det(P) = e^{i\theta} \det(P)$

$\Rightarrow \det(P) \neq 0$

$\Rightarrow P$ is non-singular

Let $\mathcal{U} = AP^{-1} \quad \Rightarrow \mathcal{U}$ is unique

b) $Ax = b \quad \Rightarrow \mathcal{U} P x = b \quad \Rightarrow P x = \mathcal{U}^* b$

Since P is a semi-definite Hermitian, we can use Cholesky or conj. grad. to solve.

Problem 6

Aug 2014

$$\begin{cases} u'' + \alpha u^2 = \sin(\pi x) \\ u(0) = u(1) = 0 \end{cases}$$

a) Let $u_i = u(ih)$ where $i = 1, \dots, n$ and $h = \frac{1}{n}$.

$\Rightarrow$ $u_0 = u(0)$ and $u_n = u(1)$.

Let $\vec{u} = [u_1, \dots, u_{n-1}]$

$$\Rightarrow u''(x_i) = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \quad \text{for } i = 1, 2, \dots, n-1$$

Note: $$u''(x_1) = \frac{u_0 - 2u_1 + u_2}{h^2} = \frac{-2u_1 + u_2}{h^2}$$

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ 0 & 1 & -2 & 1 \\ & & & h^2 \end{bmatrix} \qquad F(\vec{u}) = \begin{bmatrix} \alpha u_1^2 - \sin(\pi h) \\ \alpha u_2^2 - \sin(2\pi h) \\ \vdots \\ \alpha u_{n-1}^2 - \sin((n-1)\pi h) \\ 0 \end{bmatrix}$$

$$\Rightarrow AU + F(U) = \begin{bmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ 0 & 1 & -2 & 1 \\ & & & h^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} + \begin{bmatrix} \alpha u_1^2 - \sin(\pi h) \\ \alpha u_2^2 - \sin(2\pi h) \\ \vdots \\ \alpha u_{n-1}^2 - \sin((n-1)\pi h) \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

b) Recall Newton's method for mult. dim. systems:

$$\vec{x}_{n+1} = \vec{x}_n - \left(DG(\vec{x}_n)\right)^{-1}\left(G(\vec{x}_n)\right)$$

where, in this case, $G(\vec{x}_n) = A\vec{x}_n + F(\vec{x}_n)$

$$\Rightarrow DG(\vec{x}_n) = DG\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} = \begin{bmatrix} \nabla g_1 \\ \nabla g_2 \\ \vdots \\ \nabla g_n \end{bmatrix} = \begin{bmatrix} -\frac{2}{h^2} + \alpha 2 u_1 & 1/h^2 & & 0 \\ 1/h^2 & -\frac{2}{h^2} + \alpha 2 u_2 & 1/h^2 & \\ & \ddots & \ddots & \ddots \\ 0 & 1/h^2 & -\frac{2}{h} + \alpha 2 u_n & 1/h^2 \\ & & & 1 \end{bmatrix}$$

$\Rightarrow DG(\vec{x}_n)$ is non-singular so we can find its inverse and have second order convergence.