Fall 2013 Scientific Computation Comprehensive Examination

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 motivation.

1. Use the SVD to find matrix $B \in \mathbb{R}^{m\times m}$ that has the same determinant absolute value as $A \in \mathbb{R}^{m\times m}$, and best approximates A in the Frobenius norm,

$$\min_{\det B = |\det A|} \|A - B\|_F .$$

2. The Lanczos algorithm is a simplification of the Arnoldi iteration (Algorithm 1 below) for general $A \in \mathbb{C}^{m\times m}$, $b \in \mathbb{C}^m$

Algorithm 1

b arbitrary, $q_1 = b/\|b\|$
for $n = 1, 2, 3, \ldots$
  $v = A q_n$
  for $j = 1$ to n
    $h_{jn} = q_j^* v$
    $v = v - h_{jn} q_j$
  $h_{n+1,n} = \|v\|$
  $q_{n+1} = v/h_{n+1,n}$

for the special case when $A \in \mathbb{R}^{m\times m}$ and $A = A^T$ (symmetric A).

a) Write out the Lanczos algorithm in a computationally efficient form.

b) Present an analogous algorithm for the case $A = -A^T$ (skew-symmetric A).

3. Let f be the nonlinear function with zero x^* given by

$$f(x, y) = \begin{pmatrix} \cos x + e^y - 2 \\ e^{-x} + \sin y - 1 \end{pmatrix}, \quad x^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Consider the iteration

$$A x_{n+1} = -f(x_n), \quad A = \begin{bmatrix} 0 & \alpha \\ \alpha & 0 \end{bmatrix}.$$

a. Assuming x_0 is close to x^*, determine for which α the iterations converge.

b. Write out the Newton's method for this function and comment on its convergence.

4. Consider the following scheme for solving the ODE $y'(t) = f(y(t))$,

$$y_{n+1} = y_n + h\,(\alpha\, f(y_n) + \beta\, f(y_{n-1})).$$

Assume that the mesh is uniform with step size h, and $y_0 = y(0)$, $y_1 = y(h)$. This scheme is derived from the numerical integration formula

$$y_{n+1} = y_n + \int_{t_n}^{t^{n+1}} p(t)\, dt,$$

where $p(t)$ is the interpolating polynomial satisfying $p(t_n) = f_n = f(t_n, y_n)$ and $p(t_{n-1}) = f_{n-1} = f(t_{n-1}, y_{n-1})$.

a. Find α and β.

b. What is the local truncation error of this method?

c. Is this method convergent?

5. Consider the problem of constructing a polynomial approximation g of an analytic function $f\colon [a,b] \to \mathbb{R}$, using 4 precomputed values $(x_i, y_i = f(x_i))$, $i = 1, \ldots, 4$.

a. How should x_i be chosen to ensure that the error

$$\varepsilon = \max_{a \leqslant x \leqslant b} |f(x) - g(x)|$$

is minimized?

b. Present a tight upper bound for the error ε, and evaluate it for $f(x) = \exp(x)$ on $[a,b] = [-1,1]$. Is the upper bound attained in this case?

6. Consider the numerical quadrature of integrals of form

$$\int_0^h \sqrt{x}\, f(x)\, \mathrm{d}x = A\, f(a h) + B\, f(b h) + C h^p, \tag{1}$$

with $h > 0$, and $f\colon [0,h] \to \mathbb{R}$ an analytic function.

a. Determine a, b, A, B corresponding to two-point Gauss-Legendre quadrature

$$\int_{-1}^{+1} F(x)\, \mathrm{d}x \cong F\left(-\frac{1}{\sqrt{3}}\right) + F\left(\frac{1}{\sqrt{3}}\right).$$

Present possible deficiencies of this approach (perhaps based upon a counter-example).

b. Determine alternative values a, b, A, B such that the order of the quadrature method p is as high as possible. Compute C for this case.

Problem 1

$$\min_{\det B = |\det A|} \|A-B\|_F = \min_{\det B = |\det A|} \sqrt{\sum_{i,j=1}^{m} |a_{ij}-b_{ij}|^2}$$

Or $\|A-B\|_F = \sqrt{Tr((A-B)\overline{(A-B)}^T)}$

$= \sqrt{Tr((A-B)(A-B)^T)} \quad \because A, B \in \mathbb{R}^{m \times m}$

$\uparrow$ Need to minimize the trace

If $A = U \Sigma V$

$\det(A) = \text{sign}(\det U) \cdot \text{sign}(\det V) \det(\Sigma)$

$= \text{sgn}(\det U)\, \text{sgn}(\det V) \prod_{j=1}^{m} \lambda_{jj}$

$\Rightarrow \det(B) = \prod_{j=1}^{m} \lambda_{jj}$

$\Rightarrow B = \tilde{U} \Sigma \tilde{V}^T$ where $\det(\tilde{U}) \cdot \det(\tilde{V}) = +1$

If $\det(A) \geq 0$, our job is easy, $B = A$. So we need only consider the case $\det(A) < 0$.

$A - B = \bar{U} \bar{\Sigma} \bar{V}^T$

$\sqrt{Tr(A-B)(A-B)^T} = \sqrt{Tr(\bar{\Sigma}^2)}$

?

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Problem 2

a) Given $A = A^T$.

$H_n = Q_n^T A Q_n$

$h_{ij} = q_i^T A q_j = (q_i^T A q_i)^T = q_j^T A^T q_i = q_j^T A q_i = h_{ji}$

$\Rightarrow H_n$ is symmetric $\Rightarrow H_n$ is tridiag

$$\hat{H}_n = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ & & \beta_{n-1} & \alpha_n \\ & & & \beta_n \end{bmatrix}$$

Algorithm (Lanczos Iteration)

β_0; $q_1 = \frac{b}{\|b\|}$

for $n = 1, 2, \ldots, m$

$v = Aq_n$

$\alpha_n = q_n^* v$ ← get rid of these for part b

$v = v - \alpha_n q_n - \beta_{n-1} q_{n-1}$

$\beta_n = \|v\|$

$q_{n+1} = \frac{v}{\beta_n}$

end

b) Will get $\alpha_j = 0$

Problem 3

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a) $A x_{n+1} = -f(x_n)$

$x_{n+1} = -A^{-1} f(x_n)$

where $A = \begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix} \Rightarrow A^{-1} = \begin{pmatrix} 0 & 1/\alpha \\ 1/\alpha & 0 \end{pmatrix}$.

For conv, we want $e_{n+1} < e_n$. Sps $x_0 = \begin{pmatrix} \varepsilon \\ \varepsilon \end{pmatrix}$

$$x_1 = -\begin{pmatrix} 0 & 1/\alpha \\ 1/\alpha & 0 \end{pmatrix}\begin{pmatrix} \cos(\varepsilon) + e^{\varepsilon} - 2 \\ e^{-\varepsilon} + \sin(\varepsilon) - 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\alpha}(2 - \cos(\varepsilon) - e^{\varepsilon}) \\ 1/\alpha\,(1 - e^{-\varepsilon} - \sin(\varepsilon)) \end{pmatrix}$$

$$x_{2n+1} = \left(\frac{1}{\alpha}\right)^{2n+1} \begin{pmatrix} 2 - \cos(\varepsilon) - e^{\varepsilon} \\ 1 - e^{-\varepsilon} - \sin(\varepsilon) \end{pmatrix}$$

$$x_{2n} = (1/\alpha)^{2n} \begin{pmatrix} e^{-\varepsilon} + \sin(\varepsilon) - 1 \\ \cos(\varepsilon) + e^{\varepsilon} - 2 \end{pmatrix}$$

To ensure $x_n \to x^* = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ we need $(1/\alpha)^n \to < \infty$

$\therefore \alpha \geq 1$

b) Recall mult. dim Newton's method: $\vec{x}_{n+1} = \vec{x}_n - (Df(\vec{x}_n))^{-1} f(\vec{x}_n)$

$$f(\vec{x}) = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} \cos x + e^{y} - 2 \\ e^{-x} + \sin y - 1 \end{pmatrix}$$

$$Df(\vec{x}) = \begin{pmatrix} \nabla f_1 \\ \nabla f_2 \end{pmatrix} = \begin{pmatrix} -\sin x & e^{y} \\ -e^{-x} & \cos y \end{pmatrix}$$

$$\vec{x}_{n+1} = \vec{x}_n - \begin{pmatrix} -\sin x_n & e^{y_n} \\ -e^{-x_n} & \cos y_n \end{pmatrix}^{-1} \begin{pmatrix} \cos x_n + e^{y_n} - 2 \\ e^{-x_n} + \sin y_n - 1 \end{pmatrix}$$

It has second order convergence

Problem 4

$$y_{n+1} = y_n + h(\alpha f(y_n) + \beta f(y_{n-1})) \quad \text{where} \quad y' = f$$

Need $\int_{t_n}^{t_{n+1}} p(t)\,dt \approx h(\alpha f(y_n) + \beta f(y_{n-1}))$

Newton's interpolating polynomial gives us:

$$p(t) = a_0 + a_1(t - t_n) + a_2(t - t_n)(t - t_{n-1})$$

where $a_0 = p(t_n) = f_n$

$$a_1 = \frac{p(t_{n-1}) - a_0}{t_{n-1} - t_n} = \frac{f_n - f_{n-1}}{t_n - t_{n-1}}$$

$$a_2 = \frac{f''(\xi)}{2}$$

$$p(t) = f_n + \frac{f_n - f_{n-1}}{t_n - t_{n-1}}(t - t_n) + \frac{f''(\xi)}{2}(t - t_n)(t - t_{n-1})$$

$$\Rightarrow \int_{t_n}^{t_{n+1}} p(t)\,dt = \int_{t_n}^{t_{n+1}} f_n + \frac{f_n - f_{n-1}}{t_n - t_{n-1}}(t - t_n) + \frac{f''(\xi)}{2}(t^2 - t(t_n + t_{n-1}) + t_n t_{n-1})\,dt$$

$$= f_n(t_{n+1} - t_n) + \frac{f_n - f_{n-1}}{t_n - t_{n-1}}\left(\frac{(t_{n+1} - t_n)^2}{2} - \frac{(t_n - t_n)^2}{2}\right)$$

$$+ \frac{f''(\xi)}{2}\left(\frac{t_{n+1}^3 - t_n^3}{3} - \frac{t_{n+1}^2 - t_n^2}{2}(t_n + t_{n-1}) + t_n t_{n-1}(t_{n+1} - t_n)\right)$$

Recall:
$t_{j+1} - t_j = h$

$$= h f_n + \frac{f_n - f_{n-1}}{\cancel{h}}\left(\frac{h^2}{2}\right) + \frac{f''(\xi)}{2}\left(\frac{(t_n + h)^3 - t_n^3}{3} - \frac{(t_n + h)^2 - t_n}{2}(2t_n - h) + t_n(t_n - h)h\right)$$

$$= \frac{3h}{2} f_n - \frac{h}{2} f_{n-1} + \frac{f''(\xi)}{12}\left(2(3t_n^2 h + 3t_n h^2 + h^3) - 3(2t_n h + h^2)(2t_n - \right.$$
$$6t_n^2 h - 6t_n h^2$$

$$= h\left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1}\right) + \frac{f''(\xi)}{12}\left(\cancel{6t_n^2 h} + \cancel{6t_n h^2} + 2h^3 - 12\cancel{t_n^2 h} - 3h^3 + \cancel{6t_n^2 h} - \cancel{6t_n h^2}\right.$$

$$= h\left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1}\right) - \frac{h^3}{12} f''(\xi)$$

$\rightarrow$

a) $y_{n+1} = y_n + h(\alpha f_n + \beta f_{n-1})$

$$= y_n + \int_{t_n}^{t_{n+1}} p(t)\,dt$$

$$= y_n + h\left(\tfrac{3}{2} f_n - \tfrac{1}{2} f_{n-1}\right) - \frac{h^3}{12} f''(\xi)$$

$\therefore \boxed{\alpha = 3/2 \qquad \beta = -1/2}$

b) The local truncation error is: $\boxed{-\frac{h^3}{12} f''(\xi)}$

c) Zero stable: Set $y' = 0$ and guess $y_n = r^n \Rightarrow r^{n+1} - r^n = 0$

$\Rightarrow r - 1 = 0$

$\Rightarrow y = c_1(1)^n \Rightarrow y$ is const

$\therefore$ zero-stable

Consistent: The local truncation error decays

$\therefore$ consistent

Since conv = consistent + stable, we can conclude our method is convergent.

Problem 5

a) We know: $f(x) - p(x) = \frac{1}{4!} f^{(4)}(\xi_x) \prod_{i=0}^{3} (x - x_i)$

for some $\xi_x \in [a, b]$.

$$\Rightarrow \max_{a \le x \le b} |f(x) - p(x)| \le \frac{1}{4!} \max_{a \le x \le b} |f^{(4)}(x)| \cdot \max_{a \le x \le b} \left| \prod_{i=0}^{3} (x - x_i) \right|$$

We also know $\max_{a \le x \le b} \left| \prod_{i=0}^{3} (x - x_i) \right| \ge 2^{-3}$. The minimum of this will be attained if $\prod_{i=0}^{3} (x - x_i)$ is the monic multiple of T_4; specifically $2^{-3} T_4$. The nodes will then be the roots of T_4:

$$x_i = \cos\left(\frac{2i+1}{2(4)+2} \pi\right) \qquad i = 0, 1, 2, 3$$

$$x_i = \cos\left(\frac{2i+1}{10} \pi\right)$$

b) Assuming $f(x) = e^x$ for $x \in [-1, 1]$, we have $f(x)$ is monic so:

$$|f(x) - p(x)| \le \frac{1}{2^n (n+1)!} \max_{|t| \le 1} |f^{(n+1)}(t)| \qquad \forall x$$

$$\Rightarrow \quad \varepsilon \le \frac{1}{2^3 (4!)} \max_{|x| \le 1} |e^x| = \frac{1}{8(24)} (e)$$

$$\therefore \quad \varepsilon \le \frac{e}{192}$$

Problem 6

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$$\int_0^h \sqrt{x}\, f(x)\,dx = A f(ah) + B f(bh) + C h^p$$

a) N+f y st $y(0) = -1$ and $y(h) = 1$

$$y = \frac{2}{h}x - 1 \quad \Rightarrow \quad x = \frac{h}{2}(y+1)$$
$$dx = \frac{h}{2}\,dy$$

$$I(f) = \int_0^h \sqrt{x}\, f(x)\,dx = \frac{h}{2}\int_{-1}^{1} \sqrt{\tfrac{h}{2}(y+1)}\; f\left(\tfrac{h}{2}(y+1)\right)dy = \int_{-1}^{1} F(y)\,dy = F\left(-\tfrac{1}{\sqrt{3}}\right) + F\left(\tfrac{1}{\sqrt{3}}\right)$$

$$\Rightarrow \quad F(y) = \frac{h}{2}\sqrt{\tfrac{h}{2}(y+1)}\; f\left(\tfrac{h}{2}(y+1)\right)$$

$$\Rightarrow \quad I(f) = \frac{h}{2}\sqrt{\tfrac{h}{2}(1-1/\sqrt{3})}\; f\left(\tfrac{h}{2}(1-1/\sqrt{3})\right) + \frac{h}{2}\sqrt{\tfrac{h}{2}(1+1/\sqrt{3})}\; f\left(\tfrac{h}{2}(1+1/\sqrt{3})\right)$$

$$\Rightarrow \quad A = \frac{h}{2}\sqrt{\tfrac{h}{2}(1-1/\sqrt{3})} \qquad B = \frac{h}{2}\sqrt{\tfrac{h}{2}(1+1/\sqrt{3})}$$

$$a = \tfrac{1}{2}(1-1/\sqrt{3}) \qquad b = \tfrac{1}{2}(1+1/\sqrt{3})$$

Possible deficiencies:

1) $\sqrt{x}\, f(x)$ may be hard to interpolate
2) $f(x)$ may not be defined at these pts

b) · Choose inner-product: $\langle p,q\rangle = \int_0^h \underset{\text{weight func}}{\sqrt{x}}\, p(x)q(x)\,dx$

· Find orthogonal polynomials: (Need two roots so find quad)

Basis: $\{1, x, x^2\}$

$V_1 = 1$

$V_2 = x - \dfrac{\int_0^h x^{3/2}\,dx}{\int_0^h x^{1/2}\,dx}\cdot 1 = x - \dfrac{\frac{2}{5}h^{5/2}}{\frac{2}{3}h^{3/2}} = x - \frac{3}{5}h$

$V_3 = x^2 - \dfrac{\langle x^2, v_1\rangle}{\langle v_1, v_1\rangle}\cdot V_1 - \dfrac{\langle x^2, 1\rangle}{\langle 1,1\rangle}\cdot 1 = x^2 - \frac{10h}{9}x + \frac{5h^2}{21}$

see scratch

· Find roots of V_3: (see scratch)

$x_0 = \dfrac{35h - 2h\sqrt{70}}{63}$ $\quad x_1 = \dfrac{35h + 2h\sqrt{70}}{63}$ (These are our nodes)

· Find weights:

$f(x) = 1$: $\int_0^h \sqrt{x}\,dx = \frac{2}{3}h^{3/2} = A + B$

$f(x) = x$: $\int_0^h x^{3/2}\,dx = \frac{2}{5}h^{5/2} = Ax_0 + Bx_1$

$$\begin{cases} A + B = \frac{2}{3}h^{3/2} \\ Ax_0 + Bx_1 = \frac{2}{5}h^{5/2} \end{cases}$$ Solve this for A and B

$\Rightarrow I(f) = Af(x_1) + Bf(x_2)$

To find C and p:

interpolating poly deg 2

$I(f) - Q(f) = \int_0^h \sqrt{x} f(x)\,dx - \int_0^h \sqrt{x}\, p(x)\,dx = \int_0^h (f(x) - p(x))\sqrt{x}\,dx$

from integration

$= \int_0^h \frac{f'''(\xi)}{6} \underbrace{\prod_{i=0}^{1}(x-x_i)^2}_{\leq 4} \underset{\leq 4}{\sqrt{x}}\,dx = O(h^{4+\frac{1}{2}+1}) = O(h^{11/2})$

$\Rightarrow p = 11/2$ and C is the coeff.