Scientific Computation Qualifying Examination

January 2017

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. Your goal is to present skill in formulating precise mathematical statements, and demonstrate understanding of theoretical material.

1. Assume $f(x)$ is a smooth function. Estimate $f''(0)$ using the given values $f(0)$, $f(h)$, and $f(2h)$. What is the order of your approximation formula (stencil) in terms of h?

2. (1) Assume $f(x)$ is a smooth function for $0 \le x \le 1$, discuss how to compute the integral

$$\int_0^1 \frac{f(x)}{\sqrt{x}} dx.$$

What is the order and/or degree of precision of your numerical scheme?
(2) Prove that no Gaussian quadrature formula with n nodes can be exact for all polynomials of degree $2n$ or less.

3. Present an analysis of the linear multi-step method defined by

$$x_n - 3x_{n-1} + 2x_{n-2} = h(f_n + 2f_{n-1} + f_{n-2} - 2f_{n-3}),$$

for solving the ODE $x'(t) = f(t, x)$, with $t_n = nh$, $x_n = x(t_n)$, $f_n = f(t_n, x_n)$.

4. Consider an upper Hessenberg matrix H, describe an algorithm to efficiently and stably compute its QR decomposition $H = QR$ where Q is an orthogonal matrix and R is upper triangular. What is the total number of operations of your algorithm?

5. Assume $H(x, y) = f(x) \cdot g(y)$ and consider the matrix A with entries $A_{i,j} = H(x_i, y_j)$, $i = 1, \cdots, m$ and $j = 1, \cdots, n$. Write out explicitly the singular value decomposition of A using $f(x_i)$ and $g(y_j)$. What is $rank(A)$?

Has typo

6. Let $x_j = 2\pi j/N$, for $j = 0, 1, \ldots, N-1$, and define the scalar product

$$(f, g)_N = \frac{1}{N}\sum_{j=0}^{N-1} f_j \bar{g}_j$$

with $f_j = f(x_j)$, $g_j = g(x_j)$, $\bar{z}$ the complex conjugate of $z \in \mathbb{C}$. Define column vectors $\boldsymbol{e}_k, \boldsymbol{u}, \boldsymbol{v} \in \mathbb{C}^N$, $k = 0, 1, \ldots, N-1$, with components

$$e_{jk} = \exp(ikx_j), u_j = f(x_j), v_j = (f, \vec{e}_j)_N, j = 0, 1, \ldots, N-1,$$

and the matrix $\boldsymbol{E} = \frac{1}{N}\begin{pmatrix} \vec{e}_0 & \vec{e}_1 & \ldots & \vec{e}_{N-1} \end{pmatrix} \in \mathbb{C}^{N\times N}$.

a) Prove that $\boldsymbol{v} = \boldsymbol{E}\boldsymbol{u}$.

b) How many distinct elements does $\boldsymbol{E}$ have? Is $\boldsymbol{E}$ symmetric? Is $\boldsymbol{E}$ unitary?

c) Show $\|\boldsymbol{v}\| = \frac{1}{\sqrt{N}}\|\boldsymbol{u}\|$, in the Euclidean norm on $\mathbb{C}^N$.

d) Compute the singular value decomposition of $\boldsymbol{E}$.

Problem 1

$$f(h) = f(0) + hf'(0) + \frac{h^2}{2}f''(0) + \frac{h^3}{3!}f'''(0) + \frac{h^4}{4!}f^{(4)}(0) + \dots \qquad (1)$$

$$f(2h) = f(0) + 2hf'(0) + 2h^2 f''(0) + \frac{4h^3}{3}f'''(0) + \frac{2h^4}{3}f^{(4)}(0) + \dots \qquad (2)$$

$$(2) - 2(1) \Rightarrow \quad f(2h) - 2f(h) = -f(0) + 0\cdot f'(0) + h^2 f''(0) + \Theta(h^3)$$

$$\Rightarrow f''(0) = \frac{1}{h^2}\left(f(0) - 2f(h) + f(2h) + \Theta(h^3)\right)$$

$$\Rightarrow f''(0) = \frac{1}{h^2}\left(f(0) - 2f(h) + f(2h)\right) \quad \text{has order } h \text{ accuracy}$$

OR

$$f''(0) = Af(0) + Bf(h) + Cf(2h) \qquad (1)$$

$$f(h) = f(0) + hf'(0) + \frac{h^2}{2}f''(0) + \frac{h^3}{3!}f'''(0) + \frac{h^4}{4!}f^{(4)}(0) + \dots \qquad (2)$$

$$f(2h) = f(0) + 2hf'(0) + 2h^2 f''(0) + \frac{4}{3}h^3 f'''(0) + \frac{2}{3}h^4 f^{(4)}(0) + \dots \qquad (3)$$

Subbing (2) and (3) into (1) yields:

$$f''(0) = (A+B+C)f(0) + (B+2C)hf'(0) + \left(\tfrac{1}{2}B + 2C\right)h^2 f''(0) + \left(\tfrac{1}{6}B + \tfrac{4}{3}C\right)h^3 f'''$$

$$\Rightarrow \begin{cases} A+B+C = 0 \\ B+2C = 0 \\ \tfrac{1}{2}B + 2C = \tfrac{1}{h^2} \end{cases}$$

$$\tfrac{1}{2}B = -\tfrac{1}{h^2}$$

$$B = -\tfrac{2}{h^2}$$

$$\Rightarrow C = \frac{1}{h^2} \Rightarrow A = \frac{2}{h^2} - \frac{1}{h^2} = \frac{1}{h^2}$$

Back to (1) ...

$$\Rightarrow \quad f''(0) = \frac{1}{h^2}\left(f(0) - 2f(h) + f(2h)\right) + h\left(-\tfrac{1}{3} + \tfrac{4}{3}\right)f'''(0)$$

$$\boxed{f''(0) = \frac{1}{h^2}\left(f(0) - 2f(h) + f(2h)\right) + \Theta(h)}$$

order h accuracy

a) Identify an appropriate inner-product

$$\langle p(x), q(x) \rangle = \int_0^1 \frac{p(x)q(x)}{\sqrt{x}}\,dx$$

Find an orthog basis:

$\{1, x, x^2\}$.

$u_1 = 1$

$$u_2 = x - \frac{\langle x, 1\rangle}{\langle 1, 1\rangle} 1 = x - \frac{\int_0^1 \sqrt{x}\,dx}{\int_0^1 \frac{1}{\sqrt{x}}\,dx} = x - \frac{\frac{2}{3}x^{\frac{3}{2}}\big|_0^1}{2x^{\frac{1}{2}}\big|_0^1} = x - \frac{1}{3}$$

$$u_3 = x^2 - \frac{\langle x^2, x - \frac{1}{3}\rangle}{\langle x - \frac{1}{3}, x - \frac{1}{3}\rangle}(x - \tfrac{1}{3}) - \frac{\langle x^2, 1\rangle}{\langle 1, 1\rangle}\cdot 1$$

$$= x^2 - \frac{\int_0^1 (x^{5/2} - \frac{1}{3}x^{3/2})\,dx}{\int_0^1 (x^{3/2} - \frac{2}{3}x^{1/2} - \frac{1}{4\sqrt{x}})\,dx}(x - \tfrac{1}{3}) - \frac{\int_0^1 x^{3/2}\,dx}{2} = x^2 - \frac{\frac{2}{7} - \frac{2}{15}}{\frac{2}{5} - \cancel{\frac{4}{9}} - \frac{2}{9}}(x - \tfrac{1}{3}) - \frac{1}{5}$$

$-\frac{2}{3}$

$$= x^2 - \frac{30 - 14}{42 - 70}(x - \tfrac{1}{3}) - \frac{1}{5} = x^2 + \frac{\cancel{16}\,4}{\cancel{28}\,7}(x - \tfrac{1}{3}) - \frac{1}{5} = x^2 + \frac{4}{7}x \underbrace{- \frac{4}{21} - \frac{1}{5}}_{-\frac{41}{105}}$$

Roots of u_3 = points of eval = a, b

weights: $f(x) = 1$

$f(x) = x$ ← create system of eqns to find A, B

$$\Rightarrow \int_0^1 \frac{f(x)}{\sqrt{x}}\,dx \approx A\,F(a) + B\,F(b)$$

Degree of precision = 2

b) We know that the Gaussian quad. form. is, in fact, exact for all polynomials of deg $\leq 2n-1$. So the problem must lie with the polynomial of deg $2n$.

Consider $\deg(f(x)) = n$

$$\int_a^b f^2(x)\,w(x)\,dx > 0$$

$\because$ is non-neg and can only be zero at isolated points. ($f^2(x)$ has at most $2n$ roots and w can only vanish at isolated pts by defn of the weighted func.)

But since x_i are roots for of $f(x)$ for $i = 1, 2, \ldots, n$, the quad formula gives:

$$\sum_{i=1}^{n} w_i f^2(x_i) = 0$$

Thus: $\int_a^b f^2(x)\,w(x)\,dx \neq \sum_{i=1}^{n} w_i f^2(x_i)$

so it can't be exact $\forall$ polynomials of deg $2n$.

Spring 2017

Problem 3

Let $x'(t) = f(t,x)$ where $t_n = nh$, $x_n = x(t_n)$ and $f(t_n, x_n)$.

$$x_n - 3x_{n-1} + 2x_{n-2} = h(f_n + 2f_{n-1} + f_{n-2} - 2f_{n-3})$$

Let L be a linear operator st: $Lx = \sum_{k=0}^{3}[a_k x_{n-k} - b_k h x'_{n-k}]$

Analysis means "does this meth. conv?"

where $a_0 = 1$ $a_1 = 2$ $a_2 = -3$ $a_3 = 0$

$b_0 = 1$ $b_1 = 2$ $b_2 = 1$ $b_3 = -2$

Convergence = consistency + stability

Consistency:

(N+f. local truncation error)

Taylor series about t_n: Note: $x_n' = f_n$

$$x_n - 3(x_n - hx_n' + O(h^2)) + 2(x_n - 2hx_n' + O(h^2))$$

$$= hf_n + 2h(f_n + h\partial_t f_n + h(\partial_y f_n)\underbrace{y_n'}_{f_n} + O(h^2))$$

$$+ h(f_n + O(h)) - 2h(f_n + O(h))$$

$O(1)$: $x_n - 3x_n + 2x_n = 0$ ✓

$O(h)$: $3f_n - 4f_n = f_n + 2f_n + f_n - 2f_n$

$-f_n \neq 2f_n$ inconsistent

$\Rightarrow$ Method is 1st order when it convs

Stability:

Is the method zero-stable? Check $x' = 0$. Does the soln stay bounded?

Guess: $x_n = r^n$

$$r^n - 3r^{n-1} + 2r^{n-2} = 0$$

$$r^2 - 3r + 2 = 0$$

$$r = 1, 2 \quad \Rightarrow \quad x_n = c_1(1)^n + c_2(2)^n$$

Is $\lim_{n\to\infty} x_n < \infty$? No

$\therefore$ not zero-stable $\Rightarrow$ not alway conv

Problem 4

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We use Given's rotation:

$$G = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \quad \text{st} \quad G\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$

$$\Rightarrow \alpha = \sqrt{x_1^2 + x_2^2} \quad \Rightarrow \cos\theta = \frac{x_1}{\sqrt{x_1^2+x_2^2}} \qquad \sin\theta = \frac{-x_2}{\sqrt{x_1^2+x_2^2}}$$

Algorithm

$R = H;\ Q = I;$

for $j = 1:m-1$ (size $H = m \times m$)

$$\left.\begin{array}{l}
\text{if } x_1 > x_2 \\
\quad t = \frac{x_2}{x_1} \\
\quad \cos\theta = \frac{1}{\sqrt{1+t^2}} \\
\quad \sin\theta = \frac{-t}{\sqrt{1+t^2}} \\
\text{end} \\
\text{if } x_1 < x_2 \\
\quad t = \frac{x_1}{x_2} \\
\quad \cos\theta = \frac{t}{\sqrt{1+t^2}} \\
\quad \sin\theta = \frac{-1}{\sqrt{1+t^2}} \\
\text{end}
\end{array}\right\} \ast$$

$R_{j:j+1,:} = G^T R_{j:j+1,:}$ ♡

$Q_{j:j+1,:} = Q_{j:j+1,:} G$ □

Operation Count

$$\left.\begin{array}{l}
\ast - 5 \text{ ops} \\
\heartsuit - 4m \text{ ops} \\
\square - 4m \text{ ops}
\end{array}\right\} m-1 \text{ times} = (8m+5)(m-1) \sim \underline{8m^2 \text{ ops}}$$

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Problem 5

since $H(x,y) = f(x)\,g(y)$

$\Rightarrow A = \vec{f}\,\vec{g}^{T}$ where $\vec{f} = \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix}$ $\vec{g} = \begin{pmatrix} g(y_1) \\ \vdots \\ g(y_n) \end{pmatrix}$

diagnol

N+f: U, Σ, V s t $A = U \Sigma V^{T}$

orthonormal

Let $\vec{F} = \frac{\vec{f}}{\|\vec{f}\|}$ since $\vec{F}$ is only one colum it is automatical orthogonal. And by defn, it is normalized.

Let $\vec{G} = \frac{\vec{g}}{\|\vec{g}\|}$. Then G is also orthonormal.

$\Rightarrow U = \vec{F}$ and $V = \vec{G}$

Thus Σ must be the 1×1 matrix (scalar) 1.

Hence $\operatorname{rank}(A) = \operatorname{rank} \Sigma = 1$.

Problem 6

Spring 201

$$\langle f, g\rangle_N = \frac{1}{N}\sum_{j=0}^{N-1} f_j \overline{g_j}$$

$v_j = \langle f, \vec{e}_j\rangle$ $\qquad$ $e_{jk} = e^{ikx_j} \Rightarrow \vec{e}_k = \begin{pmatrix} e^{ix_k} \\ \vdots \\ e^{i(N-1)x_k} \end{pmatrix}$

$E = \frac{1}{N}(\vec{e}_0 \; \vec{e}_1 \; \dots \; \vec{e}_{N-1})$ $\qquad$ $x_k = \frac{2\pi}{N}k$

$u_j = f(x_j)$

a) $v_k = \langle f, \vec{e}_k\rangle = \frac{1}{N}\sum_{j=0}^{N-1} f_j \overline{e_{jk}} = \frac{1}{N}(f_0 \overline{e}_{0k} + f_1 \overline{e}_{1k} + \dots + f_n \overline{e}_{nk})$

$= \frac{1}{N}(\overline{e}_0 u_{0k} + \overline{e}_{1k} u_{1k} + \dots + \overline{e}_{nk} u_n)$

$= \frac{1}{N}(\overline{e}_{0k} \; \dots \; \overline{e}_{nk}) \cdot (u_0 \; \dots \; u_n)$

$= E\vec{u}$

b) $E = \frac{1}{N}(\vec{e}_0 \; \vec{e}_1 \; \dots \; \vec{e}_{N-1})$ where $e_{jk} = e^{ikx_j} = e^{ikj(\frac{2\pi}{N})} = e^{ijx_k} = e_{kj}$

$\therefore$ E is symmetric

E has no more than N distinct elts because there are only N distinct values for $e^{i\frac{2\pi}{N}n}$ $n \in \mathbb{Z}$.

$\therefore \rightarrow a_{0k} = e^0 = 1$

$$E = \begin{array}{l} \text{row 1} \\ \text{row 2} \\ \\ \\ \end{array} \begin{bmatrix} a_{00}^{=1} & a_{01}^{=1} & \dots & a_{0,N-1}^{=1} \\ 1 = a_{10} & a_{11} \neq & \dots & a_{1,N-1} \\ * & & \ddots & \vdots \\ & & & a_{N-1,N-1} \end{bmatrix}$$

$e^{2\pi/N}$ $\qquad$ $e^{\frac{2\pi}{N}(N-1)}$

In row two, there is: $1, e^{\frac{2\pi}{N}}, e^{\frac{2\pi}{N}\cdot 2}, \dots, e^{\frac{2\pi}{N}N-1}$ which are all distinct so we must have at least N distinct elts. Thus, E has exactly N distinct el~~t~~s.

$E^* = \overline{E}$ b/c E is sym

$$\overline{E}E = \frac{1}{N}\begin{bmatrix} \overline{e}_0 \\ \overline{e}_1 \\ \vdots \\ \overline{e}_{N-1} \end{bmatrix} \frac{1}{N}\begin{bmatrix} e_0 & e_1 & \cdots & e_{N-1} \end{bmatrix}$$

$$\overline{e}_K e_j = \frac{1}{N^2}\sum_{l=0}^{N-1} \overline{e_{Kl}}\, e_{jl} = \frac{1}{N^2}\sum_{l=0}^{N-1} e^{-iKl\frac{2\pi}{N}} e^{ijl\frac{2\pi}{N}} = \frac{1}{N^2}\sum_{l=0}^{N-1} e^{i\frac{2\pi}{N}l(j-K)}$$

For $j \neq K$, it is known that the sum of all N^{th} roots of unity is zero so $\overline{e}_K e_j = 0$

For $j = K$