Scientific Computation Comprehensive Examination

FALL 2015

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. Let the function $f: [-1,1] \to \mathbb{R}$ be defined as $f(x) = \sum_{k=0}^{n+1} a_k T_k(x)$, with $a_k \in \mathbb{R}$, $T_k: [-1, 1] \to \mathbb{R}$ the Chebyshev polynomial of degree k for $k = 0, 1, \ldots, n+1$. Show that the solution of the problem

$$\min_{g \in \Pi_n} \|f - g\|_\infty,$$

is $g(x) = \sum_{k=0}^{n} a_k T_k(x)$, with Π_n the space of polynomials of degree at most n.

2/3 2. Construct a spline interpolation by circular arcs of the data $\mathcal{D} = \{(x_k, y_k), k = 0, 1, \ldots, n\}$, $n \geqslant 2$, i.e., determine coefficients of the functions $(x - a_k)^2 + (y - b_k)^2 = r_k^2$, valid between points (x_{k-1}, y_{k-1}) and (x_k, y_k).

3. Determine the best piecewise linear approximations,

$$\bar{u}(x) = \begin{cases} 2\,a\,x & \text{for } 0 \le x \le 1/2 \\ 2\,a\,(1-x) & \text{for } 1/2 \le x \le 1 \end{cases}$$

of the exact solution $u(x)$ to the boundary value problem

$$-u''(x) = 8, 0 < x < 1,\ u(0) = u(1) = 0,$$

in the norms $\|v(x)\|_2 = \left(\int_0^1 |v(x)|^2\right)^{1/2}$, and $\|v(x)\|_e = \left(\int_0^1 |v'(x)|^2\right)^{1/2}$. Plot the two approximations and exact solution. Comment on the result.

√ 4. Let $A \in \mathbb{R}^{n \times n}$ be of full rank and consider the linear system of equations $My = c$, with

$$M = \begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix}, y = \begin{pmatrix} r \\ x \end{pmatrix}, c = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

a. Show that this system has a solution in which x minimizes $\|Ax - b\|_2$.

b. Determine the condition number of M in terms of the singular values of A.

c. Determine an explicit expression for M^{-1} as a block 2-by-2 matrix.

1/2 5. (a) Determine the order of convergence of the error of the quadrature formula

$$\int_0^1 f(x)\, dx \approx \frac{1}{8} f(0) + \frac{3}{8} f\left(\frac{1}{3}\right) + \frac{3}{8} f\left(\frac{2}{3}\right) + \frac{1}{8} f(1).$$

for cubic polynomials?

(b) Establish a quadrature rule that is exact for cubic polynomials and uses only two evaluations of the integrand, or show that such a quadrature rule cannot exist.

2/3 6. (a) Prove that Newton's method to find solutions of $f(x) = 0$ is first-order convergent at a multiple root.
(b) Prove that Aitken extrapolation restores second-order convergence at multiple roots.
(c) What is the order of convergence of the Aitken extrapolation at simple roots?

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Problem 1

$$f(x) = \sum_{k=0}^{n+1} a_k T_k(x) \qquad \text{where } a_k \in \mathbb{R}, \; T_k : [-1,1] \longrightarrow \mathbb{R}$$

↑ Chebyshev

$g(x) \in \Pi_n$

Wts: Best approx of $f(x)$ (deg $n+1$) is chebyshev deg n poly's.

We know Chebychev polynomials of degree m will have a smaller (max difference) uniform norm than any other monic polynomial of degree m. With this in mind consider the following polynomial:

$$Q(x) = \frac{1}{a_{n+1}}\left(f(x) - g(x)\right)$$

To minimize $\|Q\|$, we know it must be a Chebyshev polynomial w/ the same degree as Q. Note $\deg(Q) = \deg(f) = n+1 \because \deg(g) = n$.

$$\Rightarrow \quad T_{n+1}(x) = Q(x) = \frac{1}{a_{n+1}}\left(f(x) - g(x)\right)$$

$$\Rightarrow \quad g(x) = f(x) - a_{n+1} T_{n+1}$$

$$= \sum_{k=0}^{n+1} a_k T_k - a_{n+1} T_{n+1}$$

$$= \sum_{k=0}^{n} a_k T_k$$

Note: $\min\limits_{g \in \Pi_n} \|f-g\|_\infty^{k=0} = \min\limits_{g \in \Pi_n} \left(\max\limits_{x \in [-1,1]} |f-g| \right)$

Problem 3

$$\begin{cases} u''(x) = -8 & x \in (0,1) \\ u(0) = u(1) = 0 \end{cases} \Rightarrow \begin{array}{l} u'(x) = -8x + a \Rightarrow u(x) = -4x^2 + ax + b \\ u(0) = b = 0 \\ u(1) = -4 + a = 0 \end{array}$$

$u = -4x^2 + 4x$ = soln

$\bar{u} = \begin{cases} 2ax & 0 \le x \le 1/2 \\ 2a(1-x) & 1/2 \le x \le 1 \end{cases}$ = piecewise linear approx of u

a) Want to minimize $\| u - \bar{u} \|_2 = \left(\int_0^1 |u - \bar{u}|^2 \, dx \right)^{1/2}$ wrt a.

Let $I = \int_0^1 |u - \bar{u}|^2 dx$. Minimizing I will also minimize $\| u - \bar{u} \|_2$.

$$0 = \frac{dI}{da} = \frac{d}{da} \int_0^1 (u^2 - 2u\bar{u} + \bar{u}^2)\, dx$$

$$= \int_0^1 (-2u\bar{u}_a + 2\bar{u}\bar{u}_a)\, dx$$

$$= 2 \left(\underbrace{\int_0^{1/2} (\bar{u}\bar{u}_a - u\bar{u}_a)\, dx}_{I_1} + \underbrace{\int_{1/2}^1 (\bar{u}\bar{u}_a - u\bar{u}_a)\, dx}_{I_2} \right)$$

$$I_1 = \int_0^{1/2} (2ax(2x) - (-4x^2 + 4x)(2x))\, dx$$

$$= \int_0^{1/2} (4ax^2 + 8x^3 - 8x^2)\, dx$$

$$= \frac{4a}{3}x^3 + 2x^4 - \frac{8}{3}x^3 \Big|_0^{1/2} = \frac{4a}{3}\left(\frac{1}{2}\right)^3 + 2\left(\frac{1}{2}\right)^4 - \frac{8}{3}\left(\frac{1}{2}\right)^3$$

$$= \frac{a}{6} + \frac{1}{8} - \frac{1}{3} = \frac{a}{6} - \frac{5}{24}$$

$$I_2 = \int_{1/2}^1 (2a(1-x)(2(1-x)) - (-4x^2 + 4x)(2(1-x)))\, dx$$

$$= \int_{1/2}^1 (4a(1-x)^2 - 8x(1-x)^2)\, dx$$

$$= \int_{1/2}^1 (4a - 8ax + 4ax^2 - 8x + 16x^2 - 8x^3)\, dx$$

$$= 4ax - 4ax^2 + \frac{4a}{3}x^3 - 4x^2 + \frac{16}{3}x^3 - 2x^4 \Big]_{1/2}^1$$

$$= \cancel{4a} - \cancel{4a} + \frac{4a}{3} - 4 + \frac{16}{3} - 2 - \left(\underline{2a} - \underline{a} + \underline{\frac{a}{6}} - 1 + \frac{2}{3} - \frac{1}{8} \right)$$

$$= \frac{7a}{6} - a - 5 + \frac{14}{3} + \frac{1}{8} = \frac{a}{6} - \frac{1}{3} + \frac{1}{8} = \frac{a}{6} - \frac{5}{24}$$

$$0 = I_a = 2(I_1 + I_2) = 2\left(\frac{a}{6} - \frac{5}{24} + \frac{a}{6} - \frac{5}{24}\right).$$

$$0 = \cancel{2}\left(\frac{a}{3} - \frac{5}{12}\right)$$

$$\frac{a}{3} = \frac{5}{12}$$

$$\boxed{a = 5/4}$$

b) Want to minimize $\|u - \bar{u}\|_e = \left(\int_0^1 |u_x - \bar{u}_x|^2 dx\right)^{1/2}$ wrt a

Let $I = \int_0^1 |u_x - \bar{u}_x|^2 dx$. Minimizing I for a will also minimize a for $\|u - \bar{u}\|_e$

$$0 = \frac{dI}{da} = \int_0^1 2(-u_x \bar{u}_{xa} + \bar{u}_x \bar{u}_{xa})\, dx$$

$$= 2\Big(\underbrace{\int_0^{1/2} (\bar{u}_x \bar{u}_{xa} - u_x \bar{u}_{xa})\, dx}_{I_1} + \underbrace{\int_{1/2}^1 (\bar{u}_x \bar{u}_{xa} - u_x \bar{u}_{xa})\, dx}_{I_2}\Big)$$

$$I_1 = \int_0^{1/2} \big((2a)(2) - (-8x+4)(2)\big)\, dx = \int_0^{1/2} (4a + 16x - 8)\, dx$$

$$= 4ax + 8x^2 - 8x \Big|_0^{1/2} = 2ax + 2 - 4 = 2ax - 2$$

$$I_2 = \int_{1/2}^1 \big((-2a)(-2) - (-8x+4)(-2)\big)\, dx = \int_0^1 (4a - 16x + 8)\, dx$$

$$= 4ax - 8x^2 + 8x \Big|_{1/2}^1 = 4a - \cancel{8} + \cancel{8} - (2a - 2 + 4) = 2a - 2$$

$$0 = I_a = 2(I_1 + I_2) = 2(2a - 2 + 2a - 2) = 8a - 8$$

$$\Rightarrow \boxed{a = 1}$$

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Problem 4

a) $My = b$

$$\begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

$$\begin{cases} Ir + Ax = b \\ A^T r = 0 \end{cases} \Rightarrow \underbrace{A^T r}_{=0} + A^T A x = A^T b$$

$$A^T A x - A^T b = 0$$

$$A^T(Ax - b) = 0$$

This means $Ax-b$ is orthogonal to the column space of A. When this occurs, we also have that $Ax-b$ is minimized.

b) Note: This is a poorly conditioned saddle pt system

c) $\underbrace{\begin{pmatrix} B & C \\ D & E \end{pmatrix}}_{M^{-1}} \underbrace{\begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix}}_{M} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$

$$\Rightarrow \begin{cases} B + CA^T = I \\ BA = 0 & \Rightarrow B = 0 \\ D + EA^T = 0 \\ DA = I & \Rightarrow D = A^{-1} \end{cases}$$

$$\begin{cases} CA^T = I \\ A^{-1} + EA^T = 0 \end{cases} \Rightarrow \begin{aligned} &C = (A^T)^{-1} \\ &E = -A^{-1}(A^T)^{-1} = -(A^TA)^{-1} \end{aligned}$$

$$M^{-1} = \begin{pmatrix} 0 & (A^T)^{-1} \\ A^{-1} & -(A^TA)^{-1} \end{pmatrix}$$

Problem 5

a) $$E = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b \prod_{i=0}^{n-1} (x-x_i)^2 \, dx \qquad \xi \in (a,b)$$

Let $s = \frac{x-x_0}{h} \Rightarrow$

$ds = \frac{1}{h} dx \Rightarrow h\,ds = dx$

$$x - x_0 = hs$$
$$x - x_1 = x - x_0 + x_0 - x_1 = hs + h = h(s+1)$$
$$x - x_2 = x - x_0 + x_0 - x_2 = hs + 2h = h(s+2)$$
$$\vdots$$

A cubic polynomial, $n=4$

$$E = \frac{f^{(8)}(\xi)}{8!} \int_0^1 \prod_{i=0}^{3} (x-x_i)\, dx$$

$$= \frac{f^{(8)}(\xi)}{8!} \int_0^1 \left(\prod_{i=0}^{3} h(s+i)\right) h\, ds$$

$$= \frac{f^{(8)}(\xi)}{8!} \int_0^1 \left(h^4 \prod_{i=0}^{3} (s+i)\right) h\, ds$$

$$= \frac{f^{(8)}(\xi)}{8!} h^5 \int_0^1 \prod_{i=0}^{3} (s+i)\, ds$$

$$= O(h^5)$$

b) • Define inner product: $\langle p,q\rangle = \int_0^1 pq\,dx$

• Find orthogonal polynomials: $\{1, x, x^2\}$

$$v_1 = 1$$

$$v_2 = x - \frac{\langle x,1\rangle}{\langle 1,1\rangle}\cdot 1 = x - 1/2$$

$$v_3 = x^2 - \frac{\langle x^2, x-1/2\rangle}{\langle x-1/2, x-1/2\rangle}(x-1/2) - \frac{\langle x^2,1\rangle}{\langle 1,1\rangle}\cdot 1 = x^2 - x + \frac{1}{2} - \frac{1}{3}$$

$$= x^2 - x + 1/6$$

$$\int_0^1 (x^3 - \tfrac{1}{2}x^2)\,dx = \frac{1}{4} - \frac{1}{6} = \frac{1}{12}$$

$$\int_0^1 (x^2 - x + 1/4)\,dx = \frac{1}{3} - \frac{1}{2} + \frac{1}{4} = \frac{1}{12}$$

• Find roots of v_3 to get nodes

$$x_{1,2} = \frac{1 \pm \sqrt{1-4/6}}{2} = \frac{1}{2} \pm \frac{1}{2}\sqrt{1/3} = \frac{1}{2} \pm \frac{1}{2\sqrt{3}}$$

• Find weights by making exact

$$f(x)=1: \quad \int_0^1 dx = Af(x_1) + Bf(x_2)$$

$$1 = A + B$$

$$f(x)=x: \quad \int_0^1 x\,dx = Af(x_1) + B(x_1)$$

$$1/2 = A\left(\frac{1}{2} - \frac{1}{2\sqrt{3}}\right) + B\left(\frac{1}{2} + \frac{1}{2\sqrt{3}}\right)$$

$$\Rightarrow \begin{cases} A + B = 1 \\ A\left(1 - \frac{1}{\sqrt{3}}\right) + B\left(1 + \frac{1}{\sqrt{3}}\right) = 1 \end{cases} \Rightarrow A = 1 - B$$

$$(1-B)\left(1 - \frac{1}{\sqrt{3}}\right) + B\left(1 + 1/\sqrt{3}\right) = 1$$

$$\cancel{1} - \frac{1}{\sqrt{3}} - \cancel{B} + \frac{1}{\sqrt{3}}B + \cancel{B} + \frac{1}{\sqrt{3}}B = \cancel{1}$$

$$\frac{2}{\sqrt{3}}B = \frac{1}{\sqrt{3}}$$

$$B = 1/2$$

$$A = \frac{1}{2}$$

Thus our quadrature formula is:

$$\int_0^1 f\,dx = \frac{1}{2}f\left(\frac{1}{2} - \frac{1}{2\sqrt{3}}\right) + \frac{1}{2}f\left(\frac{1}{2} + \frac{1}{2\sqrt{3}}\right)$$

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Problem 6

a) $x_{n+1} = g(x_n) = x_n - \frac{f(x_n)}{f'(x_n)}$

Let α be a root of f with multiplicity 2.

$\Rightarrow f(\alpha) = f'(\alpha) = 0 \quad f''(\alpha) \neq 0$

$$e_{n+1} = x_{n+1} - \alpha = g(x_n) - \alpha = (\cancel{g(\alpha)} + \underset{\substack{\uparrow \\ \text{N+f}}}{g'(\alpha)} e_n + O(e_n^2)) - \cancel{\alpha}$$

$$g'(x) = 1 - \frac{(f')^2 - f''f}{(f')^2} = 1 - 1 + \frac{f''f}{(f')^2} = \frac{f''f}{(f')^2} \qquad (g'(\alpha) = \tfrac{0}{0} \text{ so L'Hôp})$$

$$g'(\alpha) = \frac{f'''f + f''f'}{2f'f''}\Bigg|_{x=\alpha} \overset{\text{L'Hôp}}{=} \frac{f^{(4)}f + f'''f + f'''f' + (f'')^2}{2(f'')^2 + 2f'f''}\Bigg|_{x=\alpha} = \frac{(f''(\alpha))^2}{2(f''(\alpha))^2} = \frac{1}{2} \neq 0$$

$\Rightarrow e_{n+1} = O(e_n) \Rightarrow$ First order convergent

b) Define the sequence:

$x_n^0 = x_n$

$x_n^1 = g(x_n^0)$

$x_n^2 = g(x_n^1)$

$\vdots$

$$x_{n+1} = x_n^0 - \frac{(x_n^1 - x_n^0)^2}{x_n^2 - 2x_n^1 + x_n^0} = h(x_n) = x_n - \frac{(g(x_n) - x_n)^2}{g(g(x_n)) - 2g(x_n) + x_n}$$

$$e_{n+1} = x_{n+1} - \alpha = h(x_n) - \alpha$$
$$= \cancel{h(\alpha)} + h'(\alpha)e_n + h''(\alpha)e_n^2 + \dots + \cancel{h(\alpha)}$$

If $h'(\alpha) = 0$, then this method will conv faster

$\rightarrow$

$$h'(x)\Big|_{\alpha} = 1 - \frac{2(g-x)(g'-1)\overbrace{(g(g)-2g+x)}^{=0} - \overbrace{(g-x)^2}^{=0}(g'(g)g' - 2g'+1)}{\underbrace{(g(g)-2g+x)^2}_{=0}}\Bigg|_{x=\alpha}$$

L'Hôp

$$= 1 - \frac{2(g'-1)^2\overbrace{(g(g)-2g+x)}^{=0} + 2g''\overbrace{(g-x)}^{=0}\overbrace{(g(g)-2g+x)}^{=0} + \cancel{2(g-x)(g'-1)(g'g'(g)-2g'+1)} - \left(\cancel{2(g-x)(g'-1)(g'g'(g)-2g'+1)} + \overbrace{(g-x)^2}^{=0}(g''g'(g)+(g')^2g''(g)-2g''+1)\right)}{2\underbrace{(g(g)-2g+x)}_{=0}(g'\cdot g'(g)-2g'+1)}\Bigg|_{x=}$$

L'Hôp

$$= 1 - \frac{2(g'-1)^2\cancel{(g'g'(g)-2g'+1)} + \text{stuff that goes to zero}}{2\cancel{(g'\cdot g'(g)-2g'+1)^2} + \text{''}}\Bigg|_{x=\alpha}$$

$$= 1 - \frac{2(g'(\alpha)-1)^2}{2(g'(\alpha)g'(g(\alpha)) - 2g'(\alpha)+1)} = 1 - \frac{2(g'(\alpha)-1)^2}{2(g'(\alpha)^2 - 2g'(\alpha)+1)} = 1-1=0$$

Thus we have at least second order convergence so it is higher.

c) Notice that Aitken extrapolation just gives us Steffensen's method.

$$h(x_n) = x_n - \frac{f(x_n)^2}{f(x_n+f(x_n))-f(x_n)} = x_n - \frac{f(x_n)^{\cancel{2}}}{\cancel{f(x_n)} + f'(x_n)\cancel{f(x_n)} + \underbrace{\frac{f''(\xi_n)}{2}}_{\text{const}} f(x_n)^{\cancel{2}} - \cancel{f(x_n)}}$$

$$= x_n - \frac{f(x_n)}{f'(x_n)+cf(x_n)}$$

If we assume we have a single root at α, then $f'(\alpha)\neq 0$.

$$\Rightarrow h'(x)\Big|_{\alpha} = 1 - \frac{f'(f'+cf) - f(f''+cf')}{(f'+cf)^2}\Bigg|_{x=\alpha} = 1 - \frac{f'(\alpha)^2 - 0}{f'(\alpha)^2} = 1-1=0$$

$\Rightarrow$ We have second order convergence