Scientific Computation Comprehensive Examination 01/07/14

Answer 5 questions of your choice explaining all steps that lead to a solution. Partial credit is awarded for presenting a viable solution strategy. No credit is given to computations presented without motivation.

1. Consider the multi-step method

$$y_{n+3} + \alpha_2 y_{n+2} + \alpha_1 y_{n+1} + \alpha_0 y_n = h\,(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n),$$

to approximate solutions $y(t)$ to the initial value problem $y' = f(t,\, y)$, $y(0) = y_0$, with notation $y_k \cong y(t_k)$, $t_k = kh$, $k \in \mathbb{N}$, and $h \in \mathbb{R}_+$ denoting the step size.

   a) Under what conditions on α_i, β_i, $i = 0, 1, 2$, is the global truncation error of this method of fourth order accuracy?

   b) Prove that this method cannot be both fourth order and convergent.

2. Prove the Woodbury matrix identity

$$(A + U\Sigma V)^{-1} = A^{-1} - A^{-1}U\,(\Sigma^{-1} + VA^{-1}U)^{-1}\,VA^{-1},$$

and use it to estimate the relative error in the solution of $Ax = b$ due to perturbation of the matrix A by δA, with $\|\delta A\| = \alpha\|A\|$, $\alpha \in \mathbb{R}$, $\alpha > 0$.

3. Analyze the convergence properties of Steffensen's method (root finding version)

$$x_{n+1} = x_n - \frac{f(x_n)}{g(x_n)},\; g(x) \equiv \frac{f(x + f(x)) - f(x)}{f(x)},$$

in finding solutions of the equation $f(x) = 0$, and compare with Newton's method.

4. Consider the Chebyshev polynomials $T_n(x) = \cos n\theta$, and $T_m(x) = \cos m\theta$, with $x = \cos\theta$, $n = km$, $k, m, n \in \mathbb{N}^*$. Under what condition are the roots of T_m also roots of T_n? Based on this condition, devise an efficient algorithm to compute integrals of form

$$I = \int_{-1}^{+1} \frac{f(x)}{\sqrt{1 - x^2}}\,\mathrm{d}x,$$

to within absolute error ε using pairs of Gauss-Chebyshev quadrature formulas (assume that quadrature formula weights and nodes are known).

5. By analogy to Lagrange interpolation of data $\mathcal{D} = \{(x_i,\, y_i = f(x_i)),\, i = 0, \ldots, n\}$ by the polynomial

$$p_n(x) = \sum_{i=0}^{n} \mathcal{L}_i(x)\, y_i,$$

determine polynomials $A_i(x), B_i(x)$ such that

$$h(x) = \sum_{i=0}^{n} A_i(x)\, y_i + \sum_{i=0}^{n} B_i(x)\, y_i',$$

interpolates data $\mathcal{D}$, and also $h'(x_i) = y_i' = f'(x_i)$, $i = 0, \ldots, n$.

6. Determine the rate of convergence of the Rayleigh quotient $r(v_k) = v_k^T A v_k$, to an eigenvalue of $A \in \mathbb{R}^{n\times n}$, $A = A^T$, with vectors $v_k \in \mathbb{R}^n$ given by the normalized power method $v_{k+1} = Av_k/\|Av_k\|$.

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Problem 1

a) Need to solve: $y' = f(t,y)$ where $f(t_n, y_n) = y_n'$

$\Rightarrow y_{n+3} + \alpha_2 y_{n+2} + \alpha_1 y_{n+1} + \alpha_0 y_n = h(\beta_2 y_{n+2}' + \beta_1 y_{n+1}' + \beta_0 y_n')$ use Taylor series

$$\Rightarrow y_n + 3hy_n' + \frac{9h^2}{2} y_n'' + \frac{27h^3}{3!} y_n''' + \frac{81h^4}{4!} y_n^{(4)} + \frac{(3h)^5}{5!} y^{(5)} + O(h^6)$$

$$+ \alpha_2 \left[y_n + 2hy_n' + \frac{4h^2}{2} y_n'' + \frac{8h^3}{3!} y''' + \frac{16h^4}{4!} y^{(4)} + \frac{32h^5}{5!} y^{(5)} + O(h^6) \right]$$

$$+ \alpha_1 \left[y_n + hy_n' + \frac{h^2}{2} y_n'' + \frac{h^3}{3!} y''' + \frac{h^4}{4!} y^{(4)} + \frac{h^5}{5!} y^{(5)} + O(h^6) \right]$$

$$+ \alpha_0 y_n = \beta_2 \left[hy_n + 2h^2 y_n' + \frac{4h^3}{2} y_n''' + \frac{8h^4}{6} y_n^{(4)} + \frac{16h^5}{24} y_n^{(5)} + O(h^6) \right]$$

$$+ \beta_1 \left[hy_n' + h^2 y_n'' + \frac{h^3}{2} y''' + \frac{h^4}{6} y_n^{(4)} + \frac{h^5}{24} y_n^{(5)} + O(h^6) \right.$$

$$+ h\beta_0 y_n'$$

Any combo of α_i's and β_i's that make this system true will give us forth order accuracy

$O(1)$: $y_n + \alpha_2 y_n + \alpha_1 y_n + \alpha_0 y_n = 0$

$1 + \alpha_2 + \alpha_1 + \alpha_0 = 0$

$O(h)$: $3 + 2\alpha_2 + \alpha_1 = \beta_2 + \beta_1 + \beta_0$

$O(h^2)$: $\frac{9}{2} + 2\alpha_2 + \frac{1}{2}\alpha_1 = 2\beta_2 + \beta_1$

$O(h^3)$: $\frac{9}{2} + \frac{4}{3}\alpha_2 + \frac{1}{6}\alpha_1 = 2\beta_2 + \frac{1}{2}\beta_1$

$O(h^4)$: $\frac{81}{24} + \frac{16}{24}\alpha_2 + \frac{1}{24}\alpha_1 = \frac{4}{3}\beta_2 + \frac{1}{6}\beta_1$

$O(h^5)$: $\frac{243}{120} + \frac{32}{120}\alpha_2 + \frac{1}{120}\alpha_1 = \frac{16}{24}\beta_2 + \frac{1}{24}\beta_1$

If we go for 5^{th} order accuracy then we have 6 eqns and 6 unknowns so we can solve for unique α_i's and β_i's.

(Note, if we have 5^{th} order we automatically get 4^{th} order)

b) convergence $\rightarrow$ consistent + stable

Part a gives us consistency, so we need to check stability.

Check: $y' = 0 \rightarrow y_{n+3} + \alpha_2 y_{n+2} + \alpha_1 y_{n+1} + \alpha_0 y_n = 0$

$$y_n = r^n \Rightarrow r^{n+3} + \alpha_2 r^{n+2} + \alpha r^{n+1} + \alpha_0 r^n = 0$$

$$r^3 + \alpha_2 r^2 + \alpha_1 r + \alpha_2 = 0$$

Method is stable if roots of $f(r)$, $|r_j| < 1$

$f(r) = (r - r_1)(r - r_2)(r - r_3)$

$= r^3 - r^2(r_1 + r_2 + r_3) + r(r_1 r_2 + r_2 r_3 + r_1 r_3) - r_1 r_2 r_3$

$\alpha_2 = -(r_1 + r_2 + r_3) \longrightarrow$ If $\alpha_2 > 3$, then $\exists\, r_i$ st $|r_i| > 1$

$\Rightarrow \alpha_1 = r_1 r_2 + r_2 r_3 + r_1 r_3$ *

$\alpha_0 = -r_1 r_2 r_3 \longrightarrow$ If $|\alpha_0| > 1$ then $\exists\, r_j$ st $|r_j| > 1$

W/ Mathematica: $\alpha_0 = \frac{86}{13} \rightarrow$ Not zero-stable

Would use Mathematica to solve system in part a then check conditions from *.

Problem 2

Wts: $(A+U\Sigma V)^{-1} = A^{-1} - A^{-1}U(\Sigma^{-1}+VA^{-1}U)^{-1}VA^{-1}$

$$(A+U\Sigma V)(A^{-1}-A^{-1}U(\Sigma^{-1}+VA^{-1}U)^{-1}VA^{-1})$$

$$= I - U(\Sigma^{-1}+VA^{-1}U)^{-1}VA + (U\Sigma V)A^{-1} - (U\Sigma V)A^{-1}U(\Sigma^{-1}+VA^{-1}U)^{-1}VA^{-1}$$

$$= I + U\Sigma VA^{-1} - (U(\Sigma^{-1}+VA^{-1}U)^{-1}VA^{-1} + U\Sigma VA^{-1}U(\Sigma^{-1}+VA^{-1}U)^{-1}VA^{-1})$$

$$= I + U\Sigma VA^{-1} - (U+U\Sigma VA^{-1}U)(\Sigma^{-1}+VAU)^{-1}VA^{-1}$$

$$= I + U\Sigma VA^{-1} - U\Sigma(\Sigma^{-1}+VA^{-1}U)(\Sigma^{-1}+VAU)^{-1}VA^{-1}$$

$$= I + U\Sigma VA^{-1} - U\Sigma VA^{-1}$$

$$= I$$

$\therefore$ The identity holds

Problem 3

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

Note that if α is a root of $f(x)$, that is $f(\alpha)=0$, then $h(\alpha)=\alpha$ b/c it is a fixed pt iteration. Now let $e_n = x_n - \alpha$

$$\Rightarrow e_{n+1} = x_{n+1} - \alpha = h(x_n) - h(\alpha) \underset{\substack{\uparrow \\ \text{Taylor} \\ \text{series}}}{=} \cancel{h(\alpha)} + h'(\alpha)e_n + \frac{e_n^2}{2}h''(\alpha) - \cancel{h(\alpha)}$$

Check if $h'(\alpha)=0$

$$h(x) = x - \frac{f^2(x)}{f(x+f(x)) - f(x)} \underset{\substack{\uparrow \\ \text{Taylor} \\ \text{series}}}{=} x - \frac{f^2(x)}{\cancel{f(x)} + f'(x)f(x) + \frac{1}{2}f''(\xi)f^2(x) - \cancel{f(x)}}$$

$$h(x) = x - \frac{f(x)}{f'(x) + \frac{1}{2}f''(\xi)f(x)}$$

$$h'(x) = 1 - \frac{f'(x)\left(f'(x) + \frac{1}{2}f''(\xi)f(x)\right) - f(x)\left(f''(x) + \frac{1}{2}f''(\xi)f'(x)\right)}{\left(f'(x) + \frac{1}{2}f''(\xi)f(x)\right)^2}$$

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

$\therefore$ We have at least 2^{nd} order convergence $\because$ $e_{n+1} = O(e_n^2)$

$\rightarrow$

	Newton's	Steffensen's
Conv at single roots	second order	Second order
Conv at mult roots	first order	second order
Efficiency	Needs $f'(x)$ Two evals	No $f'(x)$ Two evals

Problem 4

$T_n(x) = \cos(n\theta)$ $\quad T_m(x) = \cos(m\theta)$ $\quad$ where $\quad x = \cos(\theta)$

Note: $n = km$ $\quad$ where $\quad n, m, k \in \mathbb{N} \cup \{0\}$

Want to know if $T_m(x) = 0$, when will $T_n(x) = 0$?

Let $T_m(x) = \cos(m\theta) = 0$. If $T_n(x) = \cos(n\theta) = 0$

$\Rightarrow \cos(m\theta) = \cos(km\theta)$

$$m\theta = km\theta + 2j\pi$$

$$\theta = \frac{2j}{1-km}\pi \quad \text{or} \quad k = 1 - \frac{2j\pi}{m\theta}$$

Since $k \in \mathbb{N}^* \Rightarrow \frac{2j\pi}{m\theta} \in \mathbb{Z} \setminus \mathbb{Z}^+ \Rightarrow m\theta \mid (-2j\pi)$

divides

$$m = \left(km + \frac{2j}{\alpha}\right)$$

Problem 5

Goal: $h(x_j) = y_j$ and $h'(x_i) = y_i'$

$$h(x_j) = \sum_{i=0}^{n} A_i(x_j) y_i + \sum_{i=0}^{n} B_i(x_j) y_i'$$

$$\Rightarrow A_i(x_j) = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$

$$B_i(x_j) = 0$$

$$h'(x_j) = \sum_{i=0}^{n} A_i'(x_j) y_i + \sum B_i'(x_j) y_i'$$

$$\Rightarrow A_i'(x_j) = 0 \qquad B_i'(x_j) = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$

Let's start w/ $B_i(x_j)$.

$$B_i(x) = \prod_{k=0}^{n} (x - x_k)$$

But $B_i'(x_j)$ implies : $B_i(x) = \prod_{k=0}^{n} (x - x_k) \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x-k)}{(x_i - x_k)^2} = (x - x_i) \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)}{(x_i - x_k)}$

Now we need A_i's

$$A_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} (x - x_k)$$

$$A_i'(x_j) = 0 \Rightarrow A_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)^2}{(x_i - x_k)^2} \leftarrow \text{Normalize}$$

$$\Rightarrow A_i(x) = \underbrace{\prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)^2}{(x_i - x_k)^2}}_{2n\text{-deg poly}} q(x)$$

Need polynomial to be degree $2n+1$ $\because$ we have

$$\underbrace{n+1 \text{ data pts}}_{D} + \underbrace{n+1 \text{ data pts}}_{D'}$$

$$A_i(x_i) = 1 \cdot q(x_i) = 1 \qquad \text{to satisfy original cond}$$

$$A_i'(x_i) = q'(x_i) \cdot 1 + \frac{d}{dx} \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x-x_k)^2}{(x_i - x_k)^2} \Bigg|_{x = x_i} \cdot \cancel{q(x_i)}^{\,1} = 0$$

$$q'(x_i) + \sum_{\substack{k=0 \\ k \neq i}}^{n} \frac{2}{x_i - x_k} = 0$$

$$\Rightarrow q'(x_i) = - \sum_{k=0}^{n} \frac{2}{x_i - x_k}$$

$$\Rightarrow q(x) = -\left(\sum_{k=0}^{n} \frac{2}{x_i - x_k} \right) x + C$$

$$\Rightarrow q(x_i) = -\left(\sum_{k=0}^{n} \frac{2}{x_i - x_k} \right) x_i + C$$

$$\Rightarrow A_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x-x_k)^2}{(x_i - x_k)^2} \left(1 + \sum_{\substack{k=0 \\ k \neq i}}^{n} \frac{2x_i}{x_i - x_k} - \left(\sum_{\substack{k=0 \\ k \neq i}}^{n} \frac{2}{x_i - x_k} \right) x \right)$$

<u>Problem 6</u>

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$r(x) = x^T A x$

Let q_1 be our eigenvector

$$r(v_k) - r(q_1) = \cancel{r(q_1)} + \nabla r(q_1)(v_k - q_1) + \mathcal{O}(\|v_k - q_1\|^2) - \cancel{r(q_1)}$$

$$\frac{\partial r}{\partial x_k} = \frac{\partial}{\partial x_k}(x^T A x) \Rightarrow \nabla r(x) = 2Ax$$

$$= 2\lambda_1 q_1 (v_k - q_1) + \mathcal{O}(\|v_k - q_1\|^2)$$

$$= 2\lambda_1 q_1 \left(\Sigma \alpha_i^{(k)} q_i - q_1\right) + \mathcal{O}(\sim)$$

$$= 2\lambda_1 \left(\|a_1^{(k)} q_1\|^2 - \|q_1\|^2\right) + \mathcal{O}(\sim)$$

$$= 2\lambda_1 \left(\|\alpha_1^{(k)}\| - 1\right) + \mathcal{O}(\sim)$$