Scientific Computing Comprehensive Exam - August 2012

Answer all of the following questions. Present a full motivation of your answers. Present a full explanation of the process by which your answers are derived, including any assumptions you make which are not stated in the problem.

1. Consider the iteration
$$x_{n+1} = \cos(x_n).$$
   (a) Show that the iteration converges to a fixed point independent of the initial guess x_0. Show that the convergence is linear and find its rate (coefficient of linearity).

   (b) Use Aitken's extrapolation to improve the method. Show that you get a higher order method and find C and p such that
$$\frac{E_{n+1}}{E_n^p} \to C \text{ as } n \to \infty,$$
   where $E_n = y_n - x^\star$, y_n is the n_{th} term of the improved sequence, and $x^\star$ is the fixed point.

2. Consider a non-singular $n \times n$ lower-triangular matrix L, show that L^{-1} is also lower-triangular. Describe an algorithm for computing L^{-1} and discuss its number of operations.

3. Consider an explicit method of the form
$$y_{n+1} = y_{n-s} + \sum_{j=0}^{s} \beta_j f^{n-j}$$
   for solving the ODE initial value problem $y'(t) = f(t, y(t))$, $y(0) = y_0$, where for each s, $\beta_0, \cdots, \beta_s$ are chosen to create an optimal (highest possible) order method.

   (a) For which s is this method stable?

   (b) Find the coefficients $\beta_0, \cdots, \beta_s$ for $s = 2$.

4. Consider integrals of the form
$$\int_0^h \frac{f(x)}{\sqrt{x}} dx$$
   where $f(x)$ is the input function.

   (a) Consider a three point stencil
$$\int_0^h \frac{f(x)}{\sqrt{x}} dx \approx h\left(c_0 f(0) + c_1 f(\frac{h}{2}) + c_2 f(h)\right).$$

Find c_0, c_1, c_2 to maximize the "degree of precision" and find C and p in the error

$$E(h) = \int_0^h \frac{f(x)}{\sqrt{x}} - h\left(c_0 f(0) + c_1 f(\frac{h}{2}) + c_2 f(h)\right) \approx Ch^p + o(h^p).$$

(b) Using this stencil, find an error bound for approximating

$$\int_0^h \sqrt{\sin(x)}dx$$

using a suitable definition of $f(x)$.

(c) What is the error bound if this stencil is applied to the integral

$$\int_0^h x dx$$

using a suitable definition of $f(x)$?

5. (a) Assume $\frac{1}{2} < x < 1$, describe an algorithm to approximate $\sqrt{x}$ using the "shifted" Chebyshev polynomial

$$\sqrt{x} \approx p_m(x) = \sum_{k=0}^{m} c_k \tilde{T}_k(x),$$

where $\tilde{T}_k$ is the classical Chebyshev polynomial T_k shifted and scaled onto the interval $[1/2, 1]$. For a given error tolerance ϵ, discuss numerical criteria for finding m and c_k such that $|\sqrt{x} - p_m(x)| < \epsilon$. How does the error decay as a function of m?

(b) Assume the $n \times n$ matrix D is symmetric positive definite, and all its eigenvalues λ_i satisfy $\frac{1}{2} < \lambda_i < 1$. Define $\sqrt{D} = U\Sigma^{\frac{1}{2}}U^T$ where D has the SVD decomposition $D = U\Sigma U^T$. Estimate $\|\sqrt{D}v - p_m(D)v\|$ for a given vector v satisfying $\|v\| = 1$.

(c) Assume D has only 3 distinct (multiple) eigenvalues $\frac{1}{2} < \lambda_1 < \lambda_2 < \lambda_3 < 1$. Can you improve the algorithm developed in (a) and (b)?

6. Consider the boundary value problem (BVP) $B(a, b)$ defined by

$$\begin{cases} -u''(x) + p(x)u(x) = q(x) \text{ for } x \in (a, b), \\ u(a) = u_a, u(b) = u_b. \end{cases}$$

(a) Discretize the above BVP using a fourth-order accurate finite difference approximation. Denote the discretization by $B_h(a, b)$. Determine the computational complexity (operation count, memory usage) of solving $B_h(a, b)$.

(b) Consider the BVPs $B(a, x_r)$, $B(x_l, b)$ with $a < x_l < x_r < b$. Devise an algorithm to construct the solution of $B_h(a, b)$ from solutions of $B_h(a, x_r)$, $B_h(x_l, b)$. Discuss various possibilities for choosing the overlap region (x_l, x_r).

(c) Compare the computational complexity of solving $B_h(a, b)$ using the method in (a) versus that in (b).

Problem 1

a) $x_{n+1} = \cos(x_n)$

We know contraction mappings have a unique fixed pt so first we decide if we have a contraction mapping.

N+f c st $d(\cos x, \cos y) \leq c\, d(x,y)$ where $c \leq 1$

(This equivalent to $\frac{\cos x - \cos y}{x - y} \leq 1$)

$$\frac{\cos(x) - \cos(y)}{x - y} = \underset{\substack{\uparrow \\ x < \chi < y}}{(\cos(\chi))'} = \sin(\chi) \leq 1$$

$\therefore\ \exists! \alpha$ st $\alpha = \cos(\alpha)$

We also know that any sequence $\{x_0, f(x_0), f(f(x_0)), \ldots\}$ will converge to the fixed pt if f is contraction mapping. Since we have shown our mapping is a contraction mapping we have our desired result.

b) $x_{n+1} = \cos(x_n) = g(x_n)$

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

$$E_{n+1} = x_{n+1} - x^* = x_n - \frac{\cos^2(x_n) - 2x_n\cos(x_n) + x_n^2}{\cos(\cos(x_n)) - 2x_n\cos(x_n) + x_n} - x^*$$

$$= E_n - \frac{\cos^2(x_n) - 2x_n\cos x_n + x_n^2}{\cos(\cos(x_n)) - 2x_n\cos(x_n) + x_n}$$

Taylor series expand around x^*

Problem 2

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Let's define $L^{-1} = (\vec{y}_1 \quad \vec{y}_2 \quad \cdots \quad \vec{y}_n)$ are column vectors.

By defn, $LL^{-1} = I$.

$$\Rightarrow \quad L (\vec{y}_1 \quad \vec{y}_2 \quad \cdots \quad \vec{y}_n) = (\vec{e}_1 \quad \vec{e}_2 \quad \cdots \quad \vec{e}_n)$$

$$\Rightarrow \quad L \vec{y}_k = \vec{e}_k$$

$$\begin{pmatrix} * & & 0 \\ & \ddots & \\ * & & * \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow k^{th} \text{ row}$$

$$\Rightarrow \quad y_{k_j} = 0 \quad \text{for} \quad j < k$$

$\Rightarrow$ L^{-1} is lower triangular

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Problem 3

$$y_{n+1} = y_{n-s} + \sum_{j=0}^{s} \beta_j f^{n-j}$$

$$\begin{cases} y' = f \\ y(0) = y_0 \end{cases}$$

a) consider $y' = 0$

$\Rightarrow \quad y_{n+1} - y_{n-s} = 0$

$\lambda^{n-s}(\lambda^{s+1} - 1) = 0$

$\lambda^{s+1} = 1$

$\Rightarrow \lambda_i =$ s+1 roots of unity

$\Rightarrow |\lambda_i| \leq 1 \quad \forall i$

$\Rightarrow$ Our method is zero-stable $\forall i$

b) $y_{n+1} = y_{n-2} + \beta_0 f_n + \beta_1 f_{n-1} + \beta_2 f_{n-2}$

$$y_{n+1} = y_n + h y_n' + \frac{h^2}{2} y'' + \frac{h^3}{6} y''' + O(h^4)$$

$$-\left(y_{n-2} = y_n - 2h y_n' + 2h^2 y'' - \frac{4h^3}{3} y''' + O(h^4) \right)$$

$$y_{n+1} - y_{n-2} = 3h y_n' - \frac{3h^2}{2} y'' + \frac{9h^3}{6} y''' + O(h^4)$$

$$f_{n-1} = y_{n-1}' = y_n' - h y_n'' + \frac{h^2}{2} y''' + O(h^3)$$

$$f_{n-2} = y_{n-2}' = y_n' - 2h y_n'' + \frac{4h^2}{2} y''' + O(h^3)$$

$$3hy_n' - \frac{3}{2}h^2 y_n'' + \frac{3}{2}h^3 y_n''' = \beta_1 y_n'$$

$$+ \cancel{\beta_2\left(y_n' - hy'' + \frac{h^2}{2}y'''\right)}$$

$$+ \beta_3\left(y_n' - 2hy'' + 2h^2 y'''\right)$$

$$\begin{cases} \beta_1 + \beta_2 + \beta_3 = 3h \\ -\beta_2 - 2\beta_3 = -\frac{3}{2}h \\ \frac{1}{2}\beta_2 + 2\beta_3 = \frac{3}{2}h \end{cases} \Bigg\} \quad -\frac{1}{2}\beta_2 = 0$$

$$\underline{\beta_2 = 0} \qquad \Rightarrow \underline{\beta_3 = \frac{3}{4}h}$$

$$\beta_1 = 3h - \frac{3}{4}h = \underline{\frac{9}{4}h = \beta_1}$$

Problem 4

$$\int_0^h \frac{f(x)}{\sqrt{x}}\,dx$$

a) $$\int_0^h \frac{f(x)}{\sqrt{x}}\,dx = h\left(c_0 f(0) + c_1 f\left(\tfrac{h}{2}\right) + c_2 f(h)\right)$$

Evaluate exactly for 3 orthogonal polynomials to create a system of equations:

$f(x)=1$: $\int_0^h x^{-1/2}\,dx = 2h^{1/2} = (c_0 + c_1 + c_2)h$

$f(x)=x$: $\int_0^h x^{1/2}\,dx = \frac{2}{3}h^{3/2} = c_1 \frac{h^2}{2} + c_2 h^2$

$f(x)=x^2$: $\int_0^h x^{3/2}\,dx = \frac{2}{5}h^{5/2} = c_1 \frac{h^3}{4} + c_2 h^3$

$$\left\{\begin{array}{l} c_0 + c_1 + c_2 = 2\frac{1}{\sqrt{h}} \\ \frac{1}{2}c_1 + c_2 = \frac{2}{3}\frac{1}{\sqrt{h}} \\ \frac{1}{4}c_1 + c_2 = \frac{2}{5}\frac{1}{\sqrt{h}} \end{array}\right. \quad \left.\right\}\ \frac{1}{4}c_1 = \frac{4}{5}\frac{1}{\sqrt{h}} \quad \Rightarrow \underline{c_1 = \frac{1}{5}\frac{1}{\sqrt{h}}}$$

$$\Rightarrow \quad c_2 = \left(\frac{2}{5} - \frac{1}{20}\right)\sqrt{h} = \underline{\frac{7}{20}\frac{1}{\sqrt{h}} = c_2}$$

$$c_0 = \left(2 - \tfrac{1}{5} - \tfrac{7}{20}\right)\sqrt{h} = \underline{\frac{29}{40}\frac{1}{\sqrt{h}} = c_0}$$

$$\int_0^h \frac{f(x)}{\sqrt{x}}\,dx = \sqrt{h}\left(\frac{29}{40}f(0) + \frac{1}{5}f(h/2) + \frac{7}{20}f(h)\right)$$

$$E(h) = \int_0^h \frac{f(x)}{\sqrt{x}}\,dx - h\left(c_0 f(0) + c_1 f(h/2) + c_2 f(h)\right)$$

$$= \int_0^h \frac{f(x)}{\sqrt{x}}\,dx - \int_0^h \frac{p(x)}{\sqrt{x}}\,dx \quad \leftarrow \text{ interpolating poly of deg 3}$$

$$= \int_0^h \frac{1}{\sqrt{x}}\left(f(x) - p(x)\right)dx$$

$$= \int_0^h \underbrace{\frac{1}{\sqrt{x}}}_{\sim h^{-1/2}} \left(\frac{f^{(4)}(\xi)}{4!} \underbrace{\prod_{i=0}^{3} (x-x_i)^2}_{\sim h^6} \right) dx = \Theta\left(h^{6-1/2+1}\right) = \Theta\left(h^{13/2}\right)$$

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

b) $f(x) = \sin x$

$\Rightarrow f^{(4)}(\xi) \leq 1$

$$E(h) \leq \int_0^h \frac{1}{\sqrt{x}} (x)(x - h/2)(x-h)\,dx$$

$$= \int_0^h \left(x^{3/2} - x^{1/2}\left(\frac{3h}{2}\right) + \frac{h^2}{2} x^{-1/2}\right) dx$$

$$= \frac{2}{5} h^{5/2} - h^{5/2} + h^{5/2} = 2/5\, h^{5/2}$$

c) $f(x) = \sqrt{x} \Rightarrow f'(x) = \frac{1}{2} x^{-1/2} \Rightarrow f''(x) = -\frac{1}{4} x^{-3/2} \Rightarrow f'''(x) = \frac{3}{8} x^{-5/2}$

$\Rightarrow f^{(4)}(x) = -\frac{15}{16} x^{-7/2}$ maximized on $[0,h]$ when $x = h$

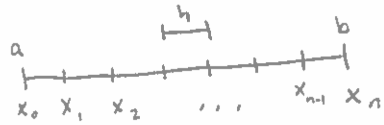
$$E(h) \leq \left| -\frac{15}{16} h^{-7/2} \int_0^h \frac{1}{\sqrt{x}} (x)(x - h/2)(x-h)\,dx \right| = \frac{15}{16} h^{-7/2} \left(\frac{2}{5} h^{5/2}\right)$$

$$= \frac{3}{8} h^{-1/2} = \frac{3}{8\sqrt{h}}$$

Problem 6

$$\begin{cases} -u''(x) + p(x)\,u(x) = q(x) & x \in (a,b) \\ u(a) = u_a\,, \quad u(b) = u_b \end{cases}$$

a)



$$u_i'' = \frac{1}{12h^2}\left(-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}\right) + \mathcal{O}(h^4)$$

$$\Rightarrow \frac{1}{12h^2}\left(u_{i+2} - 16u_{i+1} + 30u_i - 16u_{i-1} + u_{i-2}\right) + \overset{= p_i}{p(x_i)}\,u_i = \overset{= q_i}{q(x_i)} \qquad \text{for } i = 2, \dots, n-2$$

$$\frac{1}{12h^2}\begin{bmatrix} 30 & -16 & 1 & & & & 0 \\ -16 & 30 & -16 & 1 & & & \\ 1 & -16 & 30 & -16 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & & & & \\ 0 & & & & 1 & -16 & 30 \end{bmatrix}\begin{bmatrix} u_a \\ u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{n-2} \\ u_{n-1} \\ u_b \end{bmatrix} + \begin{bmatrix} p_0 u_a \\ p_1 u_1 \\ \vdots \\ \vdots \\ p_n u_b \end{bmatrix} = \begin{bmatrix} q_0 \\ q_1 \\ \vdots \\ \vdots \\ q_n \end{bmatrix}$$