Scientific Computing Comprehensive Exam - August 2017

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 Newton's method for the nonlinear equation:

$$f(x) = e^x - x - 2 = 0$$

   (a) If $(x_n)_1^\infty$ is the sequence you get when you apply Newtons method, find approximate expressions for x_1 for two cases: $x_0 = 100$, and $x_0 = -100$.

   (b) Approximately how many iterations would be required in these two cases to obtain six decimal digits of accuracy?

   (c) Show that if the initial guess is positive, Newton's method converges to the positive solution, and if the initial guess is negative, Newton's method converges to the negative solution.

2. (a) Find the coefficients and nodes of a Gaussian quadrature formula of the form

$$\int_0^1 \log(x) f(x) dx \approx A_0 f(x_0) + A_1 f(x_1)$$

   (b) Find the error in the above approximation and bound it with

$$C\|f^{(k)}\|$$

   Find C and k and find a function f such that this bound is exactly equal the error.

   (c) Prove that no Gaussian quadrature formula with n nodes can be exact for all polynomials of degree $2n$.

3. (a) Derive the multistep formula:

$$x^{n+1} = x^n + h[Af^{n+1} + Bf^n + Cf^{n-1}]$$

   What is the order of this scheme?

   (b) Determine whether the multistep method

$$x^n - x^{n-2} = h[(7/3)f^{n-1} - (2/3)f^{n-2} + (1/3)f^{n-3}]$$

   is stable and/or consistent. Is the scheme convergent?

4. The goal is to solve the boundary value problem $-u'' + \alpha u = f$ on the domain $[0, 1]$ with Dirichlet boundary conditions $u(0) = 0$ and $u(1) = 0$.

   (a) Derive the weak form for the PDE, for test functions v that are continuous and differentiable almost everywhere.

   (b) Discretize the domain using a uniformly spaced grid $x_i = i \cdot h$ where $i = 0, \ldots, N$ and $h = 1/N$. Define $N - 1$ hat functions ϕ_i that, such that for a given i, $\phi_i(x)$ is zero for $x \leq x_{i-1}$ and $x \geq x_{i+1}$, $\phi_i(x_i) = 1$ and is linear on the intervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$.

   Define our solution guess as

$$u(x) = \sum_{i=1}^{N-1} u_i \phi_i(x)$$

   Approximate f as a linear combination of the same hat functions

$$f(x) = \sum_{i=1}^{N-1} f_i \phi_i(x)$$

   Find coefficients $u_1, \ldots, u_{N-1}$ such that the u function satisfies the weak formulation of the PDE for all test functions that are spanned by $\phi_1, \ldots, \phi_{N-1}$. Do that by enforcing the weak formulation for each hat function as a test function you get $N - 1$ equations. Write down the linear system of the form

$$Au = Mf$$

   where u and f are the column vectors $(u_1, \ldots, u_{N-1})$ and $(f(x_1), \ldots, f(x_{N-1}))$.

   (c) Write down the matrix for the finite difference approximation of the same problem.

5. Consider the linear ODE

$$Y' = \begin{bmatrix} 1 & -2 \\ 5 & -5 \end{bmatrix} Y$$

   With the initial condition $Y(0) = Y_0$

   (a) Compute the analytical solution and show that it decays for $t \to \infty$.

   (b) When you use forward Euler on this ODE find the exact bound that you need for the time step for your numerical solution to also decay as $t \to \infty$

   (c) Show that if you use backward Euler the solution will decay as $t \to \infty$ independent of the time step.

Problem 1

Aug 2017

$$f(x) = e^x - x - 2 = 0$$

a) Newton's Method: $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$

$$f'(x) = e^x - 1$$

$$x_1 = x_0 - \frac{e^{x_0} - x_0 - 2}{e^{x_0} - 1} = x_0 - 1 + \frac{x_0 + 1}{e^{x_0} - 1}$$

If $x_0 = 100$

$$\Rightarrow \quad x_1 = 99 + \frac{101}{e^{100} - 1}$$

If $x_0 = -100$

$$\Rightarrow \quad x_1 = -101 + \frac{-99}{\frac{1}{e^{100}} - 1} = -100 + \frac{99e^{100}}{e^{100} - 1}$$

b) If $x_0 = 100 \Rightarrow x_1 \approx 99 \Rightarrow x_2 = 98 + \frac{100}{e^{99} - 1} \approx 98 \Rightarrow x_3 \approx 97$

$\dots \Rightarrow x_{97} \approx 3 + \frac{4}{e^3 - 1} \approx 3.25 \Rightarrow x_{98} \approx 2 + \frac{3}{e^2 - 1} \approx 2.5$

$e_{n+1} = \frac{1}{2} e_n$ for $n \geq 97$

$\frac{1}{2^{20}} \sim 10^{-7} \Rightarrow 97 + 20 = 117$

Around 117 itterations.

Similarly for $x_0 = -100$

Problem 2 Aug 2017

a) $\int_0^1 \log(x) f(x)\, dx = A_0 f(x_0) + A_1 f(x_1)$

$\uparrow$ weight func

- Define an inner product: $\langle p,q\rangle = \int_0^1 \log(x)\, p(x) q(x)\, dx$
- Find orthogonal polynomials via GS (Need quadratic to get two nodes.)

$B = \{1, x, x^2\}$

$\frac{9}{9}\cdot\frac{5}{28} - \frac{1\cdot 28}{9\cdot 28} = \frac{17}{63\cdot 4}$

$v_1 = 1$

$v_2 = x - \frac{\langle x,1\rangle}{\langle 1,1\rangle}\cdot 1 = x - \frac{1}{4}$

$v_3 = x^2 - \frac{\langle x^2, v_2\rangle}{\langle v_2, v_2\rangle} v_2 - \frac{\langle x^2, 1\rangle}{\langle 1,1\rangle} 1 = x^2 - \frac{5}{7}(x - \frac{1}{4}) - \frac{1}{9} = x^2 - \frac{5}{7}x + \frac{17}{252}$

$\langle 1,1\rangle = \int_0^1 \log(x)\,dx = x\log x\big|_0^1 - \int_0^1 dx = -1$

$\langle x,1\rangle = \int_0^1 x\log(x)\,dx = \frac{1}{2}x^2 \log x\big|_0^1 - \frac{1}{2}\int_0^1 x\, dx = -\frac{1}{4}$

$\langle x^2,1\rangle = \int_0^1 x^2\log(x)\,dx = \frac{1}{3}x^3\log x\big|_0^1 - \frac{1}{3}\int_0^1 x^2\, dx = -\frac{1}{9}$

$\langle x^2, x-\frac{1}{4}\rangle = \int_0^1 (x^3 - \frac{1}{4}x^2)\log(x)\,dx = -\frac{9}{9}\frac{1}{16} - \frac{4}{4}\cdot\frac{1}{4}(-\frac{1}{9}) = -\frac{5}{144}$

$\langle x-\frac{1}{4}, x-\frac{1}{4}\rangle = \int_0^1 (x^2 - \frac{1}{2}x + \frac{1}{16})\log(x)\,dx = -\frac{1}{9} - \frac{1}{2}(-\frac{1}{4}) + \frac{1}{16}(-1)$

$= -\frac{16\cdot 1}{16\cdot 9} + \frac{2\cdot 1\cdot 9}{2\cdot 8\cdot 9} - \frac{1\cdot 9}{16\cdot 9} = -\frac{7}{144}$

- Find nodes (roots of v_3):

$x_{1,2} = \dfrac{\frac{5}{7} \pm \sqrt{\frac{25}{49} - \frac{17}{63}}}{2} = \frac{5}{14} \pm \frac{1}{2}\sqrt{\frac{106}{49\cdot 9}} = \frac{5}{14} \pm \frac{\sqrt{106}}{42}$

- Find weights:

$f(x) = 1$: $\int_0^1 \log(x)\,dx = -1 = A_0 + A_1$

$f(x) = x$: $\int_0^1 x\log(x)\,dx = -\frac{1}{4} = A_0 x_0 + A_1 x_1$

$$\begin{cases} A_0 + A_1 = -1 \\ x_0 A_0 + x_1 A_1 = -\frac{1}{4} \end{cases}$$ solve for A_0 and A_1

b) $E(f) = \int_0^1 \log(x) f(x)\,dx - A_0 f(x_0) + A_1 f(x_1)$

Interpolating poly deg 2

$= \int_0^1 \log(x) f(x)\,dx - \int_0^1 \log(x)\, p(x)\,dx$

$= \int_0^1 \log(x)(f(x) - p(x))\,dx$

$= \int_0^1 \log(x) \left(\frac{f'''(\xi)}{6} \prod_{i=1}^{2} (x - x_i)^2 \right) dx \qquad \xi \in (0,1)$

$= \frac{f'''(\xi)}{6} \int_0^1 \log(x)\,(x - x_1)^2 (x - x_2)^2\,dx$

$\Rightarrow K = 3$ and $C = \frac{1}{6} \int_0^1 \log(x)(x - x_1)^2 (x - x_2)^2\,dx$

c) We know Gaussian quadrature with n nodes is exact $\forall$ polynomials w/ $\deg \leq 2n-1$. Thus the problem must be with polynomials of degree $2n$.

Consider $f(x)$ with degree n.

$\Rightarrow \int_a^b f^2(x)\,\omega(x)\,dx > 0$ $\because$ it is non-zero and can only be zero at isolated points.

Let x_i be the roots of $f(x)$ for $i = 1, \ldots, n$.

Then our quadrature formula gives us:

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

Thus $\int_a^b f^2(x)\,\omega(x)\,dx \neq \sum_{i=1}^{n} \omega_i f(x_i)$ so the Gaussian quadrature formula can't by exact $\forall$ polynomials of degree $2n$.

Problem 3

Aug 2017

a) $x_{n+1} = x_n + h(A f_{n+1} + B f_n + C f_{n-1})$

$$x_n + h x_n' + \frac{h^2}{2} x_n'' + \frac{h^3}{6} x_n''' + \frac{h^4}{24} x_n^{(4)} = x_n$$
$$+ Ah(x_n' + h x_n'' + \frac{h^2}{2} x_n''' + \frac{h^3}{6} x_n^{(4)}$$
$$+ Bh x_n'$$
$$+ Ch(x_n' - h x_n'' + \frac{h^2}{2} x_n''' - \frac{h^3}{6} x_n^{(4)}$$

$O(1)$: $1 = 1$

$O(h)$: $1 = A + B + C$

$O(h^2)$: $\frac{1}{2} = A - C$

$O(h^3)$: $1/6 = \frac{A}{2} + \frac{C}{2}$

$$\begin{cases} A + B + C = 1 \\ A - C = 1/2 \\ A + C = 1/3 \end{cases}$$

$A = \frac{5}{12}$ $\Rightarrow$ $C = -\frac{1}{12}$ $\Rightarrow$ $B = 1 - \frac{5}{12} + \frac{1}{12} = 2/3$

$O(h^4)$: $\frac{1}{24} \neq \frac{5}{12}\left(\frac{1}{6}\right) - \frac{1}{12}\left(-\frac{1}{6}\right) = \frac{6}{36} = \frac{1}{6}$

$\Rightarrow$ $x_{n+1} = x_n + h\left(\frac{5}{12} f_{n+1} + \frac{2}{3} f_n - \frac{1}{12} f_{n-1}\right) + O(h^4)$

order

b) $x_n - x_{n-2} = h\left(\frac{7}{3} f_{n-1} - \frac{2}{3} f_{n-2} + \frac{1}{3} f_{n-3}\right)$

Convergent = Stable + consistent

Consistent: check truncation error

$$x_n - (x_n - 2hx_n' + 2h^2 x_n'') = \frac{7}{3} h(x_n' - hx_n'' + \dots)$$
$$-\frac{2}{3} h(x_n' - 2hx_n'' + \dots)$$
$$+\frac{1}{3} h(x_n' - 3hx_n'' + \dots)$$

$\mathcal{O}(1)$: $1-1=0$ ✓

$\mathcal{O}(h)$: $2 = \frac{7}{3} - \frac{2}{3} + \frac{1}{3}$ ✓

$\mathcal{O}(h^2)$; $-2 = -\frac{7}{3} + \frac{4}{3} - 1$ ✓

So at least order h^3. Thus ~~the local truncation~~ error approaches 0 as $h \to 0$.

∴ Consistent.

Zero-Stable:

Let $x' = 0 \Rightarrow x_n - x_{n-2} = 0 \Rightarrow \lambda^{n-2}(\lambda^2 - 1) = 0 \Rightarrow \lambda = \pm 1$

$\Rightarrow x_n = c_1(-1)^n + c_2(1)^n = c_1(-1)^n + c_2$

$\Rightarrow \lim_{n\to\infty} x_n < \infty$

∴ zero-stable

Since the method is consistent and stable, it will converge

Problem 4

Aug 2017

$$\begin{cases} -u'' + \alpha u = f \\ u(0) = u(1) = 0 \end{cases} \qquad (1)$$

a) $-u'' + \alpha u - f = 0$

$\Rightarrow \int_0^1 (-u'' + \alpha u - f) v = 0$ for some func $v(x)$ that is cont and dif'ble a.e. w/ Dirchlet BC's.

$\Rightarrow \int_0^1 (-u'' v)\,dx + \int_0^1 (\alpha u v - f v)\,dx = 0$

$\Rightarrow \cancel{-u'v\Big|_0^1}^{\,0} + \int_0^1 u'v'\,dx + \int_0^1 (\alpha u v - f v)\,dx = 0$

$\Rightarrow \int_0^1 (u'v' + \alpha u v)\,dx = \int f v\,dx$

Thus the weak form is: $\begin{cases} \int_0^1 (u'v' + \alpha u v)\,dx = \int_0^1 f v\,dx \\ u(0) = u(1) = 0 \\ v(0) = v(1) = 0 \end{cases}$

b) Have $N-1$ unknowns: $u_1, u_2, \dots, u_{N-1}$. Need $N-1$ equations.

- $\emptyset_n$ might not satisfy BC's so we must enforce them (2 eqns)
- Enforce PDE w/ closed system ($N-1$ eqns)

Approximations:

$u(x) = \sum u_i \emptyset_i(x)$

$u'(x) = \sum u_i \emptyset_i'(x) = \sum u_i^{(1)} \emptyset_i(x)$ $\qquad u_i^{(1)} = \sum_{k=1}^{N-1} D_{nk} u_k$ spectral deriv

$u''(x) = \sum u_i \emptyset_i''(x) = \sum u_i^{(2)} \emptyset_i(x)$ $\qquad u_i^{(2)} = \sum_{k=1}^{N-1} K_{nk} u_k$ spectral second deriv

$\Rightarrow 0 = -u'' + \alpha u - f = \sum_{n=1}^{N-1} u_i (-\emptyset_i''(x) + \alpha \emptyset_i(x)) - \sum_{i=1}^{N-1} f_i \emptyset_i(x)$

Enforce PDE:

$$-u'' + \alpha u - f = \sum_{i=1}^{N-1} (-u_i^{(2)} + \alpha u_i)\, \phi_i(x) - f = 0$$

$$\Rightarrow \sum (-u_i^{(2)} + \alpha u_i)(\phi_i, \phi_j) = (f, \phi_j)$$

$$\sum (-u_i^{(2)} + \alpha u_i)\, \delta_{ij} \|\phi_j\|^2 = (f, \phi_j)$$

$$\sum_{i=1}^{N-1} (-K_{ji} + \alpha \delta_{ij}) \|\phi_j\|^2 u_i = (f, \phi_j)$$

$$A_{i,j+1} = (\phi_{i-1}, -\phi_j'' + \alpha \phi_j) \qquad i = 1, \dots, N-1 \qquad f_i = (\phi_i, f)$$

c) $$u''(x_i) = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \qquad u_i = u(x_i) \qquad i = 2, \dots, N-2$$

$$\Rightarrow u''(x_i) + \alpha u(x_i) = f_i$$

$$\Rightarrow \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \alpha u_i = f_i$$

$$\begin{bmatrix} 1 & -2+\alpha & 1 & & 0 \\ & 1 & -2+\alpha & 1 & \\ & & \ddots & \ddots & \ddots \\ 0 & & 1 & -2+\alpha & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ \vdots \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ f_{N-1} \end{bmatrix}$$

Problem 5

$$\begin{cases} Y' = \begin{bmatrix} 1 & -2 \\ 5 & -5 \end{bmatrix} Y \\ Y(0) = Y_0 \end{cases}$$

a) $A = \begin{bmatrix} 1 & -2 \\ 5 & -5 \end{bmatrix}$

$$\det(A - \lambda I) = (1-\lambda)(-5-\lambda) + 10 = 0$$

$$\lambda^2 + 4\lambda + 5 = 0$$

$$\lambda_{1,2} = \frac{-4 \pm \sqrt{16 - 4(5)}}{2} = -2 \pm i$$

$$\lambda_1 = -2 + i \qquad \lambda_2 = -2 - i$$

$\lambda_1 = -2 - i$:

$$\left[\begin{array}{cc|c} 1+2+i & -2 & 0 \\ 5 & -5+2+i & 0 \end{array}\right] = \left[\begin{array}{cc|c} 3+i & -2 & 0 \\ 5 & -3+i & 0 \end{array}\right] = \left[\begin{array}{cc|c} 3 & -2 + \frac{3}{5}i + \frac{1}{5} & 0 \\ 5 & -3+i & 0 \end{array}\right]$$

$$= \left[\begin{array}{cc|c} 3 & -\frac{9}{5} + \frac{3}{5}i & 0 \\ 5 & -3+i & 0 \end{array}\right] = \left[\begin{array}{cc|c} 1 & -\frac{3}{5} + \frac{1}{5}i & 0 \\ 0 & 0 & 0 \end{array}\right]$$

$$\Rightarrow u_1 = \begin{bmatrix} \frac{3}{5} - \frac{1}{5}i \\ 1 \end{bmatrix} t$$

Similary, you can find $u_2 = \begin{bmatrix} \frac{3}{5} + \frac{1}{5}i \\ 1 \end{bmatrix} t$

$$\Rightarrow Y = c_1 t e^{-(2+i)t} \begin{pmatrix} \frac{3}{5} - \frac{1}{5}i \\ 1 \end{pmatrix} + c_2 t e^{(-2+i)t} \begin{pmatrix} \frac{3}{5} + \frac{1}{5}i \\ 1 \end{pmatrix} + c_3$$

$$\lim_{t\to\infty} t e^{-(2\pm i)t} = \lim_{t\to\infty} \frac{t}{e^{2t} e^{\pm it}} \le \lim_{t\to\infty} \pm \frac{t}{e^{2t}} = 0$$

$\therefore$ the soln decays

b) Multidimentional FE:

$$y^{n+1} = y^n + h y'^n \qquad \text{where} \quad y' = AY$$

$$= y^n + hAy^n$$

$$\lim_{n\to\infty} y^{n+1} = \cancel{\lim_{n\to\infty} y^n}^{\to 0} + \lim_{n\to\infty} hAY^n = 0 \qquad \text{for} \quad h < 1$$

c) Multidimentional BE:

$$y^{n+1} = y^n + h y'^{n+1} \qquad \text{where} \quad y' = AY$$

$$y^{n+1} = y^n + hAy^{n+1}$$

$$y^{n+1} - hAy^{n+1} = y^n$$

$$y^{n+1} = y^n (I - hA)^{-1}$$

$$\Rightarrow \lim_{n\to\infty} y^{n+1} = \lim_{n\to\infty} y^n (I - hA)^{-1} = 0 \qquad \forall h$$