Department of Applied Mathematics Preliminary Examination in Numerical Analysis August 2021

Instructions. You have three hours to complete this exam. Submit solutions to four (and no more) of the following six problems. All problems have equal value.

Please start each problem on a new page. You MUST prove your conclusions or show a counter-example for all problems unless otherwise noted. Write your student ID number (not your name!) on your exam.

Problem 1: Root finding

Consider the fixed point iteration scheme

$$x_{n+1} = g(x_n).$$

- a) State the necessary conditions for the convergence of such a scheme to fixed point $x = \alpha$.
- b) Find an upper bound for the absolute error $|\alpha x_n|$.
- c) Derive from first principles the expression that shows the method to be *p*th order convergent.
- d) Consider the following iteration for calculating $\gamma^{1/3}$:

$$x_{n+1} = ax_n + b\frac{\gamma}{x_n^2} + c\frac{\gamma^2}{x_n^5}$$

Assuming that this iterative scheme converges for x_0 sufficiently close to $\gamma^{1/3}$ determine a, b, c such that the method has the highest possible convergence rate.

• Assume $g(x) \in \mathbb{C}^1([a, b]), g([a, b]) \subset [a, b]$, and

$$\lambda = \max_{a \le x \le b} |g'| < 1$$

then x = g(x) has a unique fixed point $\alpha \in [a, b], \forall x_0 \in [a, b]$ with $x_{n+1} = g(x_n)$ $n \ge 0$

$$\lim_{n \to \infty} x_n = \alpha,$$

and

$$\lim_{n \to \infty} \frac{\alpha - x_{n+1}}{\alpha - x_n} = g'(\alpha).$$

•

$$|\alpha - x_n| \le \frac{\lambda^n}{1 - \lambda} |x_1 - x_0|$$

• Order of convergence: If $g([a,b]) \in \mathbb{C}^p([a,b])$ for $p \ge 2$ and

$$g'(\alpha) = \dots = g^{p-1}(\alpha) = 0$$

then for x_0 sufficiently close to α

$$\lim_{n \to \infty} \frac{\alpha - x_{n+1}}{(\alpha - x_n)^p} = (-1)^{p-1} \frac{g^{(p)}(\alpha)}{p!}.$$

• First note that there are three unknowns so that we need 3 equations to uniquely determine a, b and c. We also know a-priori that the method should converge with order p = 3. We know that $\gamma^{\frac{1}{3}}$ is a fixed point so that $g(\gamma^{\frac{1}{3}}) = \gamma^{\frac{1}{3}}$ implying

$$a+b+c=1.$$

Also we will require $g'(\gamma \frac{1}{3}) = 0$ giving

$$a - 2b - 5c = 0,$$

and that $g''(\gamma \frac{1}{3}) = 0$ resulting in

6b + 30c = 0.

Solving this system yields $a = \frac{5}{9}$, $b = \frac{5}{9}$ and $c = -\frac{1}{9}$.

Problem 2: Quadrature

Consider $\{p_i(x)\}_{i=0}^{\infty}$, a family of orthogonal polynomials associated with the inner product

$$\langle f,g \rangle = \int_{-1}^{1} f(x) g(x) w(x) dx, \ w(x) > 0 \ \text{for} \ x \in (-1,1),$$

where $p_i(x)$ is a polynomial of the degree *i*. Let x_0, x_1, \ldots, x_n be the roots of $p_{n+1}(x)$. Construct an orthonormal basis in the subspace of polynomials of degree less or equal *n* such that, for any polynomial in this subspace, the coefficients of its expansion into the basis are equal to the scaled values of this polynomial at the nodes x_0, x_1, \ldots, x_n .

Start by considering $\ell_i(x)$, i = 0, ..., n, the Lagrange interpolating polynomials of degree n for the nodes $x_0, x_1, ..., x_n$. Let us compute the inner product of two such polynomials using the Gaussian quadrature, exact for the polynomials of degree less or equal 2n + 1. We have

$$\begin{aligned} \langle \ell_i, \ell_j \rangle &= \int_{-1}^1 \ell_i(x) \,\ell_j(x) \,w(x) \,dx \\ &= \sum_{k=0}^n \ell_i(x_k) \,\ell_j(x_k) \,w_k = \delta_{ij} w_i, \end{aligned}$$

where w_0, w_1, \ldots, w_n are the positive weights of the quadrature. If we now normalize the Lagrange interpolating polynomials,

$$R_i(x) = \frac{1}{\sqrt{w_i}} \ell_i(x) \,,$$

and compute

$$\langle R_i, R_j \rangle = \int_{-1}^1 R_i(x) R_j(x) w(x) dx$$

we obtain

$$\int_{-1}^{1} R_i(x) R_j(x) w(x) dx = \sum_{k=0}^{n} w_k R_i(x_k) R_j(x_k)$$
$$= \sum_{k=0}^{n} w_k \frac{1}{\sqrt{w_i}} \delta_{ik} \frac{1}{\sqrt{w_j}} \delta_{jk}$$
$$= \delta_{ij},$$

i.e., these functions form an orthonormal basis. The coefficients of a function in this subspace are computed as projections on the basis. We have

$$f_{i} = \langle R_{i}, f \rangle$$

$$= \int_{-1}^{1} f(x) R_{i}(x) w(x) dx$$

$$= \sum_{k=0}^{n} \alpha_{k} f(x_{k}) R(x_{k})$$

$$= \sum_{k=0}^{n} \alpha_{k} f(x_{k}) \frac{1}{\sqrt{\alpha_{k}}} \delta_{ik} = \sqrt{\alpha_{i}} f(x_{i}).$$

Problem 3: Numerical Linear Algebra

An algorithm (attributed to Eudoxos) generating a sequence of increasingly accurate approximations to the length of the diagonal of the unit square has been know in ancient Greece. Starting with $p_0 = q_0 = 1$, and defining the iteration as $p_{n+1} = p_n + q_n$, and $q_{n+1} = p_{n+1} + p_n$, n = 0, 1, 2, ...,then the ratio q_n/p_n converses to $\sqrt{2}$ as $n \to \infty$.

- (a) Prove convergence of this algorithm using the power method.
- (b) Give an expression that determines how many iterations are needed in order to achieve the accuracy

$$\left|\sqrt{2} - \frac{q_n}{p_n}\right| \le 10^{-8}?$$

(a) Writing the iteration in a matrix form, we have

$$\left(\begin{array}{c}p_{n+1}\\q_{n+1}\end{array}\right) = \left(\begin{array}{cc}1&1\\2&1\end{array}\right) \left(\begin{array}{c}p_n\\q_n\end{array}\right).$$

Computing eigenvalues and eigenvectors of the matrix, we obtain

$$\lambda_1 = 1 + \sqrt{2}, \quad \lambda_2 = 1 - \sqrt{2},$$

and

and to find n such that

$$x_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1 \end{pmatrix}, \quad x_2 = \begin{pmatrix} -1/\sqrt{2} \\ 1 \end{pmatrix}$$

Since $\lambda_1 > |\lambda_2|$, iterations of the power method will converge to the eigenvector $x_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1 \end{pmatrix}$, so that the ratio $q_{\infty}/p_{\infty} = 1/(1/\sqrt{2}) = \sqrt{2}$.

(b) In order to estimate the number of iterations, we need to compute the ratio

$$\frac{\frac{|\lambda_2|}{\lambda_1}}{\left(\frac{|\lambda_2|}{\lambda_1}\right)^n} \le 10^{-8}.$$

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Problem 4: Interpolation/Approximation

- (a) Let $f : [a, b] \to \mathbb{R}$ be a smooth function. Given the points $a < x_0 < x_1 < \cdots < x_n < b$, show there is a unique polynomial that interpolates the data $(x_i, f(x_i)), i = 0, \dots, n$.
- (b) Let $\epsilon > 0$ and consider the three data values $(0, f(0)), (\epsilon, f(\epsilon))$ and (1, f(1)). Let q be the polynomial that arises as the limit of the second order polynomial interpolant of the data as $\epsilon \to 0$.

What is the degree of q?

What data (if any) does q interpolate?

What data (if any) does q' interpolate?

(c) Given the points $a < x_0 < x_1 < \cdots < x_n < b$, denote by Ψ the function

$$\Psi(x) = \sum_{j=0}^{n} c_j e^{jx}$$

such that

$$\Psi(x_i) = f(x_i), \quad i = 0, \dots, n$$

Is the choice of interpolations constants c_0, \ldots, c_n unique? Provide justification for your answer.

- (a) Existence is equivalent to uniqueness here. To show uniqueness, assume that there are two distinct polynomials p(x) and q(x) of degree n such that $p(x_i) = q(x_i) = f(x_i)$. Then define m(x) = p(x) q(x). The polynomial m(x) is of degree n and we know that $m(x_i) = p(x_i) q(x_i) = 0$ for all x_i . In other words, the polynomial of degree n has at least n + 1 roots. The only way that this can be true is if m(x) = 0 for all $x \in [a, b]$. Thus p(x) = q(x).
- (b) This problem is easy if we use the Newton basis.

$$p_{\epsilon}(x) = f(0) + xf[0,\epsilon] + x(x-\epsilon)f[0,\epsilon,1]$$

or equivalently

$$p_{\epsilon}(x) = f(0) + x \frac{f(\epsilon) - f(0)}{\epsilon} + x(x - \epsilon) \left(f(1) - f(0) - \frac{f(\epsilon) - f(0)}{\epsilon} \right)$$

Take the limit $\epsilon \to 0$ to get

$$q(x) = f(0) + xf'(0) + x^2(f(1) - f(0) - f'(0)).$$

Thus q(x) is a polynomial of degree 2 that interpolates (0, f(0)) and (1, f(1)). The derivative of q'(x) interpolates (0, f'(0)).

(c) Let **A** denote the matrix with entries $A_{i,j} = e^{jx_i}$. Then the interpolation problem is equivalent to finding the vector $\mathbf{c} = (c_0, \ldots, c_n)^T$ such that

$$\mathbf{Ac} = (f(x_0), \dots, f(x_n))^T.$$

The matrix \mathbf{A} is a Vandermonde matrix and this is invertible since the points are distinct. Thus the constant vector \mathbf{c} is unique.

Problem 5: Numerical ODE

Consider the following method

$$y_{n+1} = y_n + \frac{h}{2} \left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}) \right], \tag{1}$$

for $n = 1, 2, 3, \ldots$, which approximate the solution of ordinary differential equations of the form

$$y' = f(x, y).$$

- (a) Determine the order of the method in equation (1).
- (b) State the conditions required for the method to be convergent.
- (c) Determine if the method is convergent.
- (d) Determine the region of absolute stability for (1).
- (e) State what is required for a method to be A-stable.
- (f) Is this method in equation (1) A-stable?

(a) We utilize Taylor's expansion for this problem.

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \frac{h^3}{3!}y^{(3)}(x) + \cdots$$

From the ODE, we know that f(x, y) = y'. Thus

$$f(x+h,y(x+h)) = y'(x+h) = y'(x) + hy''(x) + \frac{h^2}{2}y^{(3)}(x) + \frac{h^3}{3!}y^{(4)}(x) + \cdots$$

Plugging these expansions into the truncation error formula given by

$$\frac{y_{n+1} - y_n - \frac{h}{2} \left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}) \right]}{h}$$

then collecting like terms, we find that the coefficients for the y(x), y'(x) and y''(x) terms are 0. Thus the order of convergence of the method is $O(h^2)$.

- (b) A multistep method is convergent if it consistent and zero stable. A method is consistent if the truncation error goes to 0 are $h \to 0$. A method is zero stable if the roots of the zero polynomial lie within the unit disc in the complex plane and any roots on the unit circle have multiplicity one.
- (c) Since the truncation error goes to 0 as $h \to 0$, the method is consistent.

The zero polynomial for (1) is p(z) = z - 1 which has root z = 1. Thus this method is also zero stable and convergent.

(d) To determine the region of absolute stability, we apply the method to the model problem $y' = \lambda y$. The algorithm reads

$$\left(1 - \frac{h\lambda}{2}\right)y_{n+1} = \left(1 + \frac{h\lambda}{2}\right)y_n$$
$$y_{n+1} = \frac{\left(1 + \frac{h\lambda}{2}\right)}{\left(1 - \frac{h\lambda}{2}\right)}y_n$$

or

$$y_{n+1} = \frac{\left(1 + \frac{h\lambda}{2}\right)}{\left(1 - \frac{h\lambda}{2}\right)} y_n$$

The method is absolutely stable for $h\lambda$ such that

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$$\left|\frac{\left(1+\frac{h\lambda}{2}\right)}{\left(1-\frac{h\lambda}{2}\right)}\right| < 1.$$

(e) A method is A-stable if the region of absolute stability includes the entire left half complex plane. i.e. all $h\lambda$ such that $\operatorname{Real}(h\lambda) < 0$.

(g) Yes. The inequality
$$\left|\frac{\left(1+\frac{z}{2}\right)}{\left(1-\frac{z}{2}\right)}\right| < 1$$
 is satisfied for all z such that $\operatorname{Real}(z) < 0$.

Problem 6: Numerical PDE

Given the one-dimensional diffusion equation

$$\partial_t u = \partial_{xx} u$$

consider the following fully discretized scheme

$$U(x,t+k) - \frac{1}{2} (\mu - \xi) \left[U(x-h,t+k) - 2U(x,t+k) + U(x+h,t+k) \right] = U(\ell,n) + \frac{1}{2} (\mu + \xi) \left[U(x-h,t) - 2U(x,t) + U(x+h,t) \right]$$
(2)

 $\mu = k/h^2$ and $\xi = \text{constant}$.

- (a) Use Von Neumann analysis to obtain the stability condition that relates the allowable time step k and space step h.
- (b) Show that a Taylor expansion of (2) results in

$$\begin{aligned} k\partial_t u + \sum_{j=2}^\infty \frac{k^j}{j!} \partial_t^j u - \frac{1}{2} \left(\mu - \xi\right) \left[\sum_{i=2}^\infty \sum_{j=1}^\infty (1 + (-1)^i) \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \right] = \\ \mu h^2 \partial_x^2 u + \mu \left[\sum_{i=4}^\infty (1 + (-1)^i) \frac{h^i}{i!} \partial_x^i u \right] \end{aligned}$$

a) Assume

$$U(x,t) = \zeta^{t/k} e^{\mathrm{i}\omega x}$$

To get

$$\zeta \left[1 - \frac{1}{2} \left(\mu - \xi \right) 2(\cos(\omega h) - 1) \right] = 1 + \frac{1}{2} \left(\mu + \xi \right) \left[2(\cos(\omega h) - 1) \right]$$

simplifying to

$$\zeta = \frac{1 + \frac{1}{2} (\mu + \xi) 2(\cos(\omega h) - 1)}{1 - \frac{1}{2} (\mu - \xi) 2(\cos(\omega h) - 1)}$$

Given

$$\omega h \in [-\pi, \pi] \quad \Rightarrow \quad (\cos(\omega h) - 1) \in [-2, 0]$$

Thus $-1 \leq \zeta \leq 1 \quad \Rightarrow$

$$-1 + (\mu - \xi) \left(\cos(\omega h) - 1 \right) \le 1 + (\mu + \xi) \left(\cos(\omega h) - 1 \right) \le 1 - (\mu - \xi) \left(\cos(\omega h) - 1 \right)$$

Hence upper limit

$$2\mu(\cos(\omega h) - 1) \le 0 \quad \Rightarrow \quad \mu \ge 0$$

unconditionally stable. NB lower limit implies

$$-\zeta(\cos(\omega h) - 1) \le 1 \quad \Rightarrow \quad \zeta \le \frac{1}{1 - \cos(\omega h)}$$

b.) Let

$$\begin{split} U(x,t+k) &= \sum_{j=0}^{\infty} \frac{k^j}{j!} \partial_t^j u \\ U(x-h,t+k) &= \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} (-1)^i \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \\ U(x+h,t+k) &= \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \\ U(x,t) &= u(x,t) \\ U(x-h,t) &= \sum_{i=0}^{\infty} (-1)^i \frac{h^i}{i!} \partial_x^i u \\ U(x+h,t) &= \sum_{i=0}^{\infty} \frac{h^i}{i!} \partial_x^i u \end{split}$$

Thus

$$\begin{split} \sum_{j=0}^{\infty} \frac{k^{j}}{j!} \partial_{t}^{j} u &- \frac{1}{2} \left(\mu - \xi \right) \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} (-1)^{i} \frac{h^{i}}{i!} \frac{k^{j}}{j!} \partial_{x}^{i} \partial_{t}^{j} u - 2 \sum_{j=0}^{\infty} \frac{k^{j}}{j!} \partial_{t}^{j} u + \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{h^{i}}{i!} \frac{k^{j}}{j!} \partial_{x}^{i} \partial_{t}^{j} u \right] = u(x,t) + \frac{1}{2} \left(\mu + \xi \right) \left[\sum_{i=0}^{\infty} (-1)^{i} \frac{h^{i}}{i!} \partial_{x}^{i} u - 2u(x,t) + \sum_{i=0}^{\infty} \frac{h^{i}}{i!} \partial_{x}^{i} u \right] \end{split}$$

$$\begin{split} \sum_{j=0}^{\infty} \frac{k^{j}}{j!} \partial_{t}^{j} u &- \frac{1}{2} \left(\mu - \xi \right) \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} (1 + (-1)^{i}) \frac{h^{i}}{i!} \frac{k^{j}}{j!} \partial_{x}^{i} \partial_{t}^{j} u - 2 \sum_{j=0}^{\infty} \frac{k^{j}}{j!} \partial_{t}^{j} u \right] &= \\ u(x,t) &+ \frac{1}{2} \left(\mu + \xi \right) \left[\sum_{i=0}^{\infty} (1 + (-1)^{i}) \frac{h^{i}}{i!} \partial_{x}^{i} u - 2 u(x,t) \right] \end{split}$$

Eliminate u(x,t)

$$\sum_{j=1}^{\infty} \frac{k^j}{j!} \partial_t^j u - \frac{1}{2} \left(\mu - \xi\right) \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u - 2 \sum_{j=0}^{\infty} \frac{k^j}{j!} \partial_t^j u \right] = \frac{1}{2} \left(\mu + \xi\right) \left[\sum_{i=0}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \partial_x^i u - 2u(x, t) \right]$$

Separate out i = 0 on both sides

$$\begin{split} \sum_{j=1}^{\infty} \frac{k^j}{j!} \partial_t^j u &- \frac{1}{2} \left(\mu - \xi \right) \left[\sum_{i=1}^{\infty} \sum_{j=0}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \right] = \\ & \frac{1}{2} \left(\mu + \xi \right) \left[\sum_{i=1}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \partial_x^i u \right] \end{split}$$

First contributing occurs at i = 2

$$\begin{split} \sum_{j=1}^{\infty} \frac{k^j}{j!} \partial_t^j u &- \frac{1}{2} \left(\mu - \xi \right) \left[\sum_{i=2}^{\infty} \sum_{j=0}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \right] = \\ & \frac{1}{2} \left(\mu + \xi \right) \left[\sum_{i=2}^{\infty} (1 + (-1)^i) \frac{h^i}{i!} \partial_x^i u \right] \end{split}$$

This arrives at the required relation

$$\begin{aligned} k\partial_t u + \sum_{j=2}^\infty \frac{k^j}{j!} \partial_t^j u - \frac{1}{2} \left(\mu - \xi\right) \left[\sum_{i=2}^\infty \sum_{j=1}^\infty (1 + (-1)^i) \frac{h^i}{i!} \frac{k^j}{j!} \partial_x^i \partial_t^j u \right] = \\ + \mu h^2 \partial_x^2 u + \mu \left[\sum_{i=4}^\infty (1 + (-1)^i) \frac{h^i}{i!} \partial_x^i u \right] \end{aligned}$$

or