DEPARTMENT OF APPLIED MATHEMATICS

PRELIMINARY EXAMINATION IN NUMERICAL ANALYSIS

[redacted]

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Submit solutions to four (and no more) of the following six problems. Justify all your answers.

Root finding

Consider a function $f \in C^{\infty}$ in a neighborhood of its root $f(x^*) = 0$.

1. Show that if x^* is a simple root, i.e. $f'(x^*) \neq 0$, then the Newton's method converges quadratically in some neighborhood of x^*.

2. Determine the rate of convergence of the Newton's method if the root has multiplicity m, where $m \geq 2$.

Solution:

One of possible solutions is to cast the Newton's method as a fixed point iteration and apply appropriate theorems, i.e. consider a fixed point iteration for the function

$$\phi(x) = x - \frac{f(x)}{f'(x)}.$$

If the root is simple, we have

$$\phi'(x) = \frac{f(x) f''(x)}{(f'(x))^2}$$

and

$$\phi'(x^*) = 0.$$

Also we have

$$\phi''(x) = \frac{f''(x)}{f'(x)} - f(x)\left(2\frac{(f''(x))^2}{(f'(x))^3} - \frac{f'''(x)}{(f'(x))^2}\right)$$

and

$$\phi''(x^*) = \frac{f''(x^*)}{f'(x^*)} \neq 0$$

so that the convergence is quadratic.

If the root has multiplicity $m \geq 2$ then, in the neighborhood of x^*, the function f has the form,

$$f(x) = (x - x^*)^m g(x),$$

where $g(x^*) \neq 0$. Therefore, in the neighborhood of x^*, we have

$$\phi'(x) = \frac{g(x)\left(m(m-1)g(x) + (x-y)\left(2mg'(x) + (x-y)g''(x)\right)\right)}{\left(mg(x) + (x-x^*)g'(x)\right)^2}$$

so that

$$\phi'(x^*) = \frac{m-1}{m} \neq 0.$$

The iteration is convergent since

$$\phi'(x^*) < 1$$

but the rate is linear and no longer quadratic.

Numerical Quadrature

Consider a subspace $\mathscr{P}_{N-1}$ of polynomials of degree $N-1$ on the interval $[-1,1]$ and associated inner product

$$\langle f,g\rangle = \int_{-1}^{1} f(x)g(x)dx. \tag{0.1}$$

(1) Using the minimal number of nodes, construct a discrete inner product identical to (0.1) on $\mathscr{P}_{N-1}$. Prove that the two inner products coincide on $\mathscr{P}_{N-1}$.

(2) Construct an orthonormal basis in $\mathscr{P}_{N-1}$ such that in this basis the coefficients of expansion of polynomials in $\mathscr{P}_{N-1}$ are given by the scaled values of these polynomials at the nodes. (Hint: use in your construction the Lagrange interpolating polynomials and the discrete inner product).

Solution:

1. The nodes are the N zeros of the Legendre polynomial $P_N(x)=0$ and the weights of those of the corresponding Gaussian quadrature. Using these nodes and weights define

$$\langle f,g\rangle_d = \sum_{j=1}^{N} w_j f(x_j)g(x_j).$$

Since the degree of the product $f\cdot g$ does not exceed $2N-2$, this Gaussian quadrature is exact (in fact, for all polynomials up to and including the degree $2N-1$).

2. Construct Lagrange interpolating polynomials $l_i(x)$ on the nodes x_i, $i=1,\dots N$, $P_N(x_i)=0$,

$$l_i(x) = \prod_{k=1,k\neq i}^{N} \frac{x-x_k}{x_i-x_k},$$

so that $l_i(x_j)=\delta_{ij}$ (where δ_{ij} is the Kronecker symbol).

Let us show that the Legendre polynomials that form a basis in $\mathscr{P}_{N-1}$ may all be written as a linear combination of $R_i(x)=l_i(x)/\sqrt{w_j}$, $i=1,\dots,N$. We compute the coefficients of the expansion

$$P_m(x) = \sum_{i=1}^{N} a_i^m R_i(x),$$

by integrating as follows,

$$\int_{-1}^{1} P_m(x)P_k(x)dx = \sum_{i=1}^{N} a_i^m \int_{-1}^{1} R_i(x)P_l(x)dx = \sum_{i=1}^{N} a_i^m \sum_{j=1}^{N} w_j R_i(x_j)P_k(x_j) = \sum_{j=1}^{N} a_j^m \sqrt{w_j}P_k(x_j).$$

Since the matrix $P_k(x_j)$, $k=0,\dots,N-1,\ j=1,\dots,N$ is non-singular, the coefficients a_j^m exists and are unique, so that R_i indeed form a basis. We also have

$$\int_{-1}^{1} R_i(x)R_k(x)dx = \sum_{j=1}^{N} w_j R_i(x_j)R_k(x_j) = \sum_{j=1}^{N} \delta_{ij}\delta_{kj} = \delta_{ik},$$

showing that the basis is orthonormal. Consider $f\in\mathscr{P}_{N-1}$and its expansion into this basis,

$$f(x) = \sum_{i=1}^{N} f_i R_i(x).$$

By evaluating at the nodes, we have

$$f(x_j) = f_j/\sqrt{w_j},$$

or $f_j=\sqrt{w_j}f(x_j)$.

Interpolation/Approximation

(1) Show that the function

$$\frac{e^{i\theta}-\overline{\alpha}}{1-\alpha e^{i\theta}},\ \ \alpha\neq 0,$$

is a unimodular (Blaschke) factor, i.e.

$$\left|\frac{e^{i\theta}-\overline{\alpha}}{1-\alpha e^{i\theta}}\right| = 1 \text{ for } \theta\in[0,2\pi]. \tag{0.2}$$

(2) Use (0.2) to show that for $|\alpha|<1$

$$\left\|\left(1-\alpha e^{i\theta}\right)^{-1}-\sum_{j=0}^{N-1}\alpha^{j}e^{ij\theta}-\frac{\alpha^{N}}{1-\alpha\overline{\alpha}}e^{iN\theta}\right\|_{\infty}=\frac{|\alpha|^{N+1}}{1-\alpha\overline{\alpha}}$$

Solution:

1. Writing $\alpha=|\alpha|\,e^{i\psi}$ and setting $q=1-|\alpha|\,e^{i(\theta+\psi)}$, we obtain

$$\left|\frac{e^{i\theta}-\overline{\alpha}}{1-\alpha e^{i\theta}}\right|=\left|\frac{e^{i\theta}-|\alpha|\,e^{-i\psi}}{1-|\alpha|\,e^{i(\theta+\psi)}}\right|=\left|e^{i\theta}\frac{1-|\alpha|\,e^{-i(\theta+\psi)}}{1-|\alpha|\,e^{i(\theta+\psi)}}\right|=\left|e^{i\theta}\frac{\overline{q}}{q}\right|=1$$

2. We have

$$\varepsilon(\alpha,\theta)=\left(1-\alpha e^{i\theta}\right)^{-1}-\sum_{j=0}^{N-1}\alpha^{j}e^{ij\theta}-\frac{\alpha^{N}}{1-\alpha\overline{\alpha}}e^{iN\theta}=\frac{\alpha^{N}e^{iN\theta}}{1-\alpha e^{i\theta}}-\frac{\alpha^{N}}{1-\alpha\overline{\alpha}}e^{iN\theta},$$

and obtain

$$\begin{aligned}\varepsilon(\alpha,\theta)=\frac{\alpha^{N}e^{iN\theta}}{1-\alpha e^{i\theta}}-\frac{\alpha^{N}e^{iN\theta}}{1-\alpha\overline{\alpha}} &= \alpha^{N}e^{iN\theta}\left[\frac{1}{1-\alpha e^{i\theta}}-\frac{1}{1-\alpha\overline{\alpha}}\right]\\ &= \alpha^{N}e^{iN\theta}\frac{\alpha e^{i\theta}-\alpha\overline{\alpha}}{(1-\alpha e^{i\theta})(1-\alpha\overline{\alpha})}\\ &= e^{iN\theta}\frac{\alpha^{N+1}}{1-\alpha\overline{\alpha}}\frac{e^{i\theta}-\overline{\alpha}}{1-\alpha e^{i\theta}}.\end{aligned}$$

Using

$$\left|\frac{e^{i\theta}-\overline{\alpha}}{1-\alpha e^{i\theta}}\right|=1,$$

we obtain that

$$|\varepsilon(\alpha,\theta)|=\frac{|\alpha|^{N+1}}{1-\alpha\overline{\alpha}}$$

does not depend on θ and, therefore,

$$\|\varepsilon(\alpha,\theta)\|_{\infty}=\frac{|\alpha|^{N+1}}{1-\alpha\overline{\alpha}}.$$

Linear Algebra

(1) Consider two $n \times n$ matrices A and B where A is not singular. Show that the eigenvalues of AB and BA are the same.

(2) The trace of a matrix is defined as $\mathrm{Tr}(A) = \sum_{i=1}^{n} a_{ii}$, where $A = \left\{a_{ij}\right\}_{i,j=1}^{n}$. Show that

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA).$$

and that the trace is invariant under a similarity transform,

$$\mathrm{Tr}\left(X^{-1}AX\right) = \mathrm{Tr}(A).$$

Solution:

1. Since $AB = A(BA)A^{-1}$ we observe that AB and BA are similar.
2. Writing

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA).$$

explicitly, we have

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}b_{ji} = \sum_{l=1}^{n}\sum_{k=1}^{n} b_{lk}a_{kl} = \sum_{k=1}^{n}\sum_{l=1}^{n} a_{kl}b_{lk}.$$

3. Using 2. we have

$$\mathrm{Tr}\left(X^{-1}AX\right) = \mathrm{Tr}\left(AXX^{-1}\right) = \mathrm{Tr}(A).$$

ODEs

Show that the backward differentiation formula,

$$y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n = \frac{2}{3}\,h\,f\left(t_{n+2}, y_{n+2}\right),$$

gives rise to a convergent method. State and use appropriate theorems to solve this problem. What is the order of this method?

Solution:

We need to show that the order of the backward differentiation formula is $p \geq 1$ and that the method is stable (i.e. the polynomial

$$\rho\left(w\right) = \frac{1}{3} - \frac{4}{3}w + w^2$$

satisfies root condition). The Dahlquist equivalence theorem then implies that the method is convergent.

Since this is a multistep method, a possible way to establish its order is by considering

$$\psi\left(t,y\right) = y\left(t+2h\right) - \frac{4}{3}y\left(t+h\right) + \frac{1}{3}y\left(t\right) - \frac{2}{3}hy'\left(t+2h\right)$$

and verifying that

$$\psi\left(t,y\right) = 0$$

for low order polynomials of the form $y = x^n$. We have for $y = 1$

$$\psi\left(t,y\right) = 0,$$

for $y = x$

$$\psi\left(t,x\right) = t + 2h - \frac{4}{3}\left(t+h\right) + \frac{1}{3}t - \frac{2}{3}h = 0$$

for $y = x^2$

$$\psi\left(t,x\right) = \left(t+2h\right)^2 - \frac{4}{3}\left(t+h\right)^2 + \frac{1}{3}t^2 - \frac{2}{3}h\left(2h+t\right)2 = 0$$

and for $y = x^3$

$$\psi\left(t,x\right) = -\frac{4}{3}h^3 \neq 0.$$

Therefore, we obtain that the backward differentiation formula has order $p = 2$. The root condition is verified by observing that

$$\rho\left(w\right) = \left(w-1\right)\left(w - \frac{1}{3}\right).$$

PDEs

Consider two initial value problems: one for the heat equation,

$$u_t = u_{xx},$$

and, another, for the wave equation written as a first order system,

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix},$$

both with the periodic boundary conditions. The spatial discretization of these equations leads to a system of ODEs. For the discretization in time, make choice between the following two ODE methods (if you can justify using both, please do so). Your choice is between the implicit midpoint method

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}\left(x_n + \frac{h}{2}, \frac{1}{2}(\mathbf{y}_n + \mathbf{y}_{n+1})\right).$$

and the explicit midpoint method (the so-called leap-frog method),

$$\mathbf{y}_{n+2} = \mathbf{y}_n + 2h\mathbf{f}(x_{n+1}, \mathbf{y}_{n+1}).$$

Provide full justification of the merits of your selection.

Solution:

Let us establish the domain of absolute stability for the two methods. By considering the test problem,

$$y' = \lambda y, \ \ \lambda \in \mathbb{C},$$

we have

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \lambda h \frac{1}{2}(\mathbf{y}_n + \mathbf{y}_{n+1}),$$

or

$$\mathbf{y}_{n+1} = \frac{1 + \lambda h \frac{1}{2}}{1 - \lambda h \frac{1}{2}} \mathbf{y}_n,$$

so that the amplification factor

$$\left| \frac{1 + \lambda h \frac{1}{2}}{1 - \lambda h \frac{1}{2}} \right| \leq 1$$

for

$$\mathscr{R}e(\lambda h) \leq 0.$$

Therefore, the implicit midpoint method is A-stable. For the explicit midpoint method, we have

$$\mathbf{y}_{n+2} = \mathbf{y}_n + 2h\lambda \mathbf{y}_{n+1} = \mathbf{y}_n + 2z\mathbf{y}_{n+1}.$$

Solving this recurrence we have

$$r^2 - 2zr - 1 = 0$$

and

$$r_1 = z + \sqrt{z^2 + 1} \quad r_2 = z - \sqrt{z^2 + 1}.$$

In order to have bounded solutions of the recurrence, the absolute values of both roots must be less or equal to 1. Since $r_1 r_2 = -1$, we obtain that z must be of the form

$$z = i\omega,$$

and

$$r_1 = i\omega + \sqrt{1 - \omega^2} \quad r_2 = i\omega - \sqrt{1 - \omega^2},$$

so that

$$|r_1| = |r_2| = 1 \quad |\omega| \leq 1.$$

Therefore, the absolute stability region for the explicit midpoint method is the interval $[-i, i]$ of the complex axis.

The spatial discretization of the heat equation should produce a negative semi-definite matrix implying that only the implicit midpoint method can be used to evolve the equation in time. On the other hand, the spatial discretization of the wave equation should preserve the eigenvalues of the matrix

$$\begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix},$$

which are pure imaginary. Given the domain of absolute stability of the two methods, both the explicit and the implicit midpoint methods can be used.