Department of Applied Mathematics

Preliminary Examination in Numerical Analysis

August 19, 2019 , 10 am – 1 pm.

Submit solutions to four (and no more) of the following six problems. Show all your work, and justify all your answers. Start each problem on a new page, and write on one side only. No calculators allowed.
Do not write your name on your exam. Instead, write your student number on each page.

Problem 1. Root finding

Consider a random variable X with continuously-differentiable probability density $p(x) > 0$. The cumulative distribution function (cdf) is $F(x) = \int_{-\infty}^{x} p(t)dt$. Note that $\lim_{x\to\infty} F(x) = 1$.

(a) Show that $F(x)$ is invertible, i.e., $F^{-1}(y)$ exists for $y \in (0,1)$.

(b) Let $x = F^{-1}(y)$. Write Newton's method to solve for x given $y \in (0,1)$ using only evaluations of the functions $p(x)$ and $F(x)$.

(c) Explain why the method is locally at least quadratically convergent for every $y \in (0,1)$.

Solution: **(a)** There are many ways to prove this. Possibly the simplest is to note first that $F(x)$ is continuous. Next, if you pick any $y \in (0,1)$ there is always an x_0 such that $F(x_0) < y$ and an x_1 such that $F(x_1) > y$ (since $\lim_{x\to-\infty} F(x) = 0$ and $\lim_{x\to\infty} F(x) = 1$). Then by the intermediate value theorem, there must be an x between x_0 and x_1 such that $F(x) = y$, i.e. $F^{-1}(y) = x$. This value of x is unique because F is strictly increasing.

(b) Define $f(x) = F(x) - y$. We are looking for a root of $f(x)$, so

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

Note that $f'(x) = p(x)$, so Newton's method becomes

$$x_{k+1} = x_k - \frac{F(x_k) - y}{p(x_k)}.$$

(c) The function $f(x) = F(x) - y$ has a smooth positive derivative $f'(x) = p(x) > 0$, so the root is simple. Newton's method converges quadratically for smooth functions with simple roots.

Problem 2. Quadrature

Consider the integral $\int_0^\infty f(x)dx$ where f is continuous, $f'(0) \neq 0$, and $f(x)$ decays like $x^{-1-\alpha}$ with $\alpha > 0$ in the limit $x \to \infty$.

(a) Suppose you apply the equispaced composite trapezoid rule with n subintervals to approximate $\int_0^L f(x)dx$. What is the asymptotic error formula for the error in the limit $n \to \infty$ with L fixed?

(b) Suppose you consider the quadrature from (a) to be an approximation to the full integral from 0 to ∞. How should L increase with n to optimize the asymptotic rate of total error decay? What is the rate of error decrease with this choice of L?

(c) Make the following change of variable $x = L(1+y)/(1-y),\ \ y = (x-L)/(x+L)$ in the original integral to obtain $\int_{-1}^{1} F_L(y)dy$. Suppose you apply the equispaced composite trapezoid rule; what is the asymptotic error formula for fixed L?

(d) Depending on α, which method - domain truncation or change-of-variable - is preferable?

Solution: **(a)** The asymptotic error formula for the equispaced composite trapezoid rule is

$$E_n[f] \sim \frac{1}{12}\left(\frac{L}{n}\right)^2 [f'(0) - f'(L)].$$

(b) The domain truncation error is

$$\int_L^\infty f(x)\mathrm{d}x \sim \frac{L^{-\alpha}}{\alpha}.$$

We want to match the domain truncation error and the quadrature error, so

$$\frac{1}{\alpha L^\alpha} = \frac{1}{12}\left(\frac{L}{n}\right)^2 [f'(0) - f'(L)].$$

$f'(L) \to 0$ as $L \to \infty$, so it is subdominant; the dominant balance is

$$\frac{1}{\alpha L^\alpha} \sim \frac{f'(0)}{12}\left(\frac{L}{n}\right)^2.$$

Solving for L we find

$$L \sim \left(\frac{12n^2}{\alpha f'(0)}\right)^{1/(2+\alpha)}.$$

With this choice the total error scales as

$$\left(\frac{12n^2}{f'(0)}\right)^{-\alpha/(2+\alpha)}$$

as $n \to \infty$. Answers without prefactors are accepted $L \sim n^{2/(2+\alpha)}$ and error $\sim n^{2\alpha/(2+\alpha)}$.

(c) After change of variables the integrand is

$$F_L(y) = \frac{2L}{(1-y)^2} f\left(L\frac{1+y}{1-y}\right).$$

The asymptotic error formula is

$$E_n[F_L] \sim \frac{1}{12}\left(\frac{2}{n}\right)^2 \left[F_L'(-1) - F_L'(1)\right].$$

Examining the expression for $F_L(y)$ it is evident that it might have a singularity at $y = 1$, if f does not decay quickly enough. Since $f(x) \sim x^{-1-\alpha}$ then

$$F_L'(y) \sim 4L\frac{(y-\alpha)(1-y)^\alpha}{(1-y^2)^2(1+y)^\alpha}.$$

From this expression it's clear that to avoid infinite $F_L'(1)$ we need $\alpha \geq 2$. If $0 < \alpha < 2$ then we simply don't have an asymptotic error formula.

(d) The domain-truncation approach leads to an error that scales as $n^{-2\alpha/(2+\alpha)}$. The rational change of variables leads to an error that scales as n^{-2}, but only for $\alpha \geq 2$. If $\alpha \geq 2$ the transformed integral has a faster rate of convergence; otherwise it is safer to use the domain truncation (or a different change of variables).

Problem 3. Linear algebra

(a) Given two self-adjoint (Hermitian) matrices, A and B, where B is a positive (or negative) definite matrix, show that the spectrum of the product of such matrices, AB, is real.

(b) Using 2×2 matrices, construct an example where the product of two real symmetric matrices does not have real eigenvalues.

Solution:

(a)

Consider the eigenvalue problem $ABx = \lambda x,\ x \neq 0$. We have $\langle ABx, Bx\rangle = \lambda\langle x, Bx\rangle$ and observe that $\langle ABx, Bx\rangle$ is real since for any y, $\langle Ay, y\rangle = \langle y, Ay\rangle = \overline{\langle Ay, y\rangle}$. Also for $x \neq 0$, $\langle x, Bx\rangle = \langle Bx, x\rangle > 0$ since B is a positive self-adjoint operator (less than zero if B is negative definite). We therefore conclude that λ is real.

(a) Alternative solution

Say B is positive definite (PD) (else use same argument as below with -B). $B^{1/2}$ then exists and is also PD (form it with same eigenvectors as for B but use square root for each eigenvalue). AB has the same eigenvalues as $B^{1/2}(AB)B^{-1/2} = B^{1/2}AB^{1/2}$ (similarity transform). The latter matrix is Hermitian, so its eigenvalues are all real.

(b)

Consider an example with

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

where the eigenvalues of both matrices are 1 and -1 (the matrices are symmetric but indefinite). It is easy to check that the eigenvalues of AB are pure imaginary, i and $-i$.

Problem 4. Interpolation / Approximation

Let function $f \in C^{n+1}[a,b]$, $|f^{(n+1)}(x)| \le M$ and $E_n(f)$ be the error of its best approximation by a polynomial of degree *n*. Show that the accuracy of the best polynomial approximation improves rapidly as the size of the interval $[a,b]$ shrinks, i.e., show that

$$E_n(f) \le \frac{2M}{(n+1)!}\left(\frac{b-a}{4}\right)^{n+1}.$$

Hint: Use the Chebyshev nodes $x_\ell = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)\cos\left(\frac{\pi}{2}\frac{2\ell+1}{n+1}\right)$ to construct a polynomial approximation of *f*.

Solution. The error term of interpolation by a polynomial of degree $n+1$ is

$$|f(x) - p(x)| \le \max_x \frac{\left|f^{(n+1)}(x)\right|}{(n+1)!}\prod_{\ell=0}^{n}(x - x_\ell),$$

where x_ℓ are the $n+1$ nodes at which the values of f are given. On the right hand side of the inequality, change variables to the interval $[-1,1]$,

$$x = x(y) = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)\,y, \quad y \in [-1,1]$$

and use the Chebyshev nodes. We obtain

$$\max_x \frac{\left|f^{(n+1)}(x)\right|}{(n+1)!}\prod_{\ell=0}^{n}(x - x_\ell) = \max_y \frac{\left|f^{(n+1)}(x(y))\right|}{(n+1)!}\prod_{\ell=0}^{n}\frac{b-a}{2}\left(y - \cos\left(\frac{\pi}{2}\frac{2\ell+1}{n+1}\right)\right)$$

and observe that

$$\prod_{\ell=0}^{n}\left(y - \cos\left(\frac{\pi}{2}\frac{2\ell+1}{n+1}\right)\right) = \frac{T_{n+1}(y)}{2^n}.$$

We arrive at

$$|f(x) - p(x)| \le \max_y \frac{\left|f^{(n+1)}(x(y))\right|}{(n+1)!}\left(\frac{b-a}{2}\right)^{n+1}\frac{|T_{n+1}(y)|}{2^n} \le \frac{2M}{(n+1)!}\left(\frac{b-a}{4}\right)^{n+1}.$$

Alternative (similar) solution:

Consider first $[a,b]=[-1,1]$. The formula for the error in Lagrange interpolation gives $|E_n(f)| \le \max_x \frac{|f^{(n+1)}(x)|}{(n+1)!}\left|\prod_{l=0}^{n}(x-x_l)\right|$. With Chebyshev nodes, $\left|\prod_{l=0}^{n}(x-x_l)\right| = \left|\frac{1}{2^n}T_{n+1}(x)\right| \le \frac{1}{2^n}$. Stretching / contracting / shifting the interval from one of length $(b-a)$ to one of length 2 does not affect function vales, it multiplies first derivatives by $\left(\frac{b-a}{2}\right)$, second derivatives by $\left(\frac{b-a}{2}\right)^2$, ... , *n*+1st derivative by $\left(\frac{b-a}{2}\right)^{n+1}$. For the original interval $[a,b]$, we thus get $|E_n(f)| \le \frac{1}{(n+1)!}\frac{1}{2^n}M\left(\frac{b-a}{2}\right)^{n+1} = \frac{2M}{(n+1)!}\left(\frac{b-a}{4}\right)^{n+1}$.

Problem 5. Numerical ODE

There exists a one parameter family of 2-stage, second order Runge Kutta methods for solving the ODE $y' = f(x, y(x))$. With step size h in the x-direction, and the parameter α arbitrary, these can be written as

$$\begin{cases} d^{(1)} = h\,f(x_n, y_n) \\ d^{(2)} = h\,f(x_n + \alpha h, y_n + \alpha d^{(1)}) \end{cases}$$

$$y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) d^{(1)} + \frac{1}{2\alpha} d^{(2)}$$

(a) Verify that these schemes, for all values of α, indeed provide second order accuracy.

Hint: Recall that $y'(x) = f(x, y(x))$, by the chain rule, implies $y''(x) = \frac{\partial f}{\partial x} + f\,\frac{\partial f}{\partial y}$.

(b) Show that these schemes, for all α, have exactly the same stability domain.

(c) Verify that this domain, along the negative real axis, extends exactly over the interval [-2,0].

Solution:

(a) Using the formulas for $d^{(1)}$ and $d^{(2)}$, we get

$$y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) hf(x_n, y_n) + \frac{h}{2\alpha}\left(f(x_n, y_n) + \alpha h \frac{\partial f}{\partial x} + \alpha h f\,\frac{\partial f}{\partial y} + O(h^2)\right)$$

$$= y_n + hf(x_n, y_n) + \frac{1}{2}h^2\left(\frac{\partial f}{\partial x} + f\,\frac{\partial f}{\partial y}\right) + O(h^3) = y_n + hy_n' + \frac{1}{2}h^2 y_n'' + O(h^3).$$

Each step has a local error $O(h^3)$, giving a second order scheme when integrated over time.

Note that Taylor expansion is our ONLY available approach for verifying an RK-method's order of accuracy. In contrast to for linear multistep methods, it is insufficient to either (i) test by applying to increasing degree monomials, or (ii) make deductions from the method's stability domain.

(b) The stability domain is obtained by applying the scheme to the ODE $y' = \lambda y$. We obtain then

$$\begin{cases} d^{(1)} = h\lambda y_n \\ d^{(2)} = h\lambda(y_n + \alpha h y_n) \end{cases}$$

and $y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) h\lambda y_n + \frac{1}{2\alpha} h\lambda(y_n + \alpha h\lambda y_n) = y_n + h\lambda y_n + \frac{1}{2}h^2\lambda^2 y_n$. Setting $h\lambda = \xi$, this is a linear recursion relation with the characteristic equation $r = 1 + \xi + \frac{1}{2}\xi^2$. The stability domain is given by all ξ (complex) such that $|r| \le 1$.

(c) Writing the stability domain equation as $r = 1 + \frac{1}{2}\xi(2 + \xi)$ shows that, for ξ real, the condition $|r| \le 1$ is satisfied precisely for $-2 \le \xi \le 0$.

Problem 6. **Numerical PDE**

(a) Verify that the PDE $\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3}$ is well posed as an initial value problem.

(b) Consider solving it numerically using the scheme

$$\frac{u(t+k,x)-u(t-k,x)}{2k} = \frac{-\frac{1}{2}u(x-2h,t)+u(x-h,t)-u(x+h,t)+\frac{1}{2}u(x+2h,t)}{h^3} .$$

Determine this scheme's stability condition.

Hint: The 2π -periodic function $f(\theta) = 2\sin\theta(1+\cos\theta)$ oscillates in between $\pm\frac{3\sqrt{3}}{2}$.

Solution:

(a) Let $u(x,t) = \alpha(t)e^{i\omega x}$. Substituting this into the PDE gives $\alpha'(t) = -i\omega^3\alpha(t)$, with the general solution $\alpha(t) = \alpha(0)e^{-i\omega^3 t}$. With both ω and *t* real, it thus holds that $|\alpha(t)| = |\alpha(0)|$, showing that no Fourier mode can grow in time.

(b) Let $u(x,t) = \eta^{t/k}e^{i\omega x}$. Substituting this into the scheme gives, after some quick simplifications $\frac{1}{2k}\left(\eta - \frac{1}{\eta}\right) = \frac{1}{h^3}\left(-\frac{1}{2}e^{-2i\omega h} + e^{-i\omega h} - e^{i\omega h} + \frac{1}{2}e^{2i\omega h}\right) = \frac{i}{h^3}\left(2\sin\omega h(-1+\cos\omega h)\right) = \frac{i}{h^3}g(\theta)$ where $g(\theta) = 2\sin\theta(-1+\cos\theta)$ and $\theta = \omega h.$ Apart from one sign, the function $f(\theta)$ in the Hint matches $g(\theta)$. We note however that $g(\theta) = f(\theta+\pi)$, so also $g(\theta)$ oscillates between $\pm\frac{3\sqrt{3}}{2}$.

As an alternative to studying this quadratic in η, we can at this point simply refer to the stability domain for leap-frog time stepping (which is the interval from –*i* to +*i* along the imaginary axis). Using the hint, we thus need $\frac{k}{h^3}\frac{3\sqrt{3}}{2} < 1$, i.e. $\frac{k}{h^3} < \frac{2}{3\sqrt{3}}$.