Course: Numerical Algorithms
Problem Set

Instructions

- This problem set contains 30 questions: 6 easy, 15 moderate, 9 difficult.
- Questions are a mix of short-answer and long-answer formats.
- Unless otherwise stated, assume IEEE double precision arithmetic and use $\varepsilon_m \approx 10^{-16}$ as a working order-of-magnitude for machine precision.

Brief Background (for standalone use)

Many numerical algorithms treat a function f as a *black box* that can be evaluated at chosen points, even when closed-form symbolic differentiation/integration is unavailable. Finite-difference differentiation and quadrature-based integration approximate calculus operations by combining evaluations of f at carefully selected points. In practice, accuracy is limited by a tradeoff between:

- *Truncation/approximation error*, which typically decreases as the step size h shrinks, and
- *Round-off/cancellation error*, which typically increases as h shrinks (because subtracting nearly equal numbers amplifies floating-point error).

Higher-order formulas often improve accuracy by canceling lower-order error terms. Gaussian quadrature goes further by choosing nodes and weights to integrate polynomials of the highest possible degree exactly with a fixed number of function evaluations.

1 Numerical Differentiation (Q1–Q10)

Q1. (**Easy**, **Short Answer**) **[3 pts]**

Define the forward-difference approximation to $f'(x)$ using a step size $h > 0$. State the leading-order truncation error in big-O notation (as $h \to 0$), assuming f is sufficiently smooth.

Q2. (**Moderate**, **Long Answer**) **[7 pts]**

Let $f(x) = x^2 + e^x + \ln x + \sin x$ (domain $x > 0$).

(a) Compute $f'(x)$ analytically.

(b) At $x = 0.5$, compute the forward-difference approximation

$$D_f(h) = \frac{f(x+h) - f(x)}{h}$$

for $h = 10^{-2}$ and $h = 10^{-5}$ (a calculator is allowed). Report values to at least 6 significant digits.

(c) Briefly explain why *decreasing* h does not necessarily improve the numerical estimate indefinitely.

Q3. (**Difficult**, **Long Answer**) **[11 pts]**

Consider the forward-difference derivative estimate $D_f(h) = \frac{f(x+h)-f(x)}{h}$. Assume:

- truncation error scales like $c_1 h$ for some constant c_1 depending on derivatives of f at x;
- the function evaluation has floating-point perturbation of size $\mathcal{O}(\varepsilon_m)$, leading to a round-off term that scales like $c_2\varepsilon_m/h$ in the final quotient.

Task: derive a total error model of the form

$$E(h) \approx c_1 h + c_2 \frac{\varepsilon_m}{h},$$

and then minimize this model over $h > 0$ to obtain:

(a) the optimal scaling of h in terms of ε_m;

(b) the corresponding optimal achievable accuracy scaling in terms of ε_m.

Q4. (**Moderate**, **Short Answer**) **[6 pts]**

Using the error model from Q3, suppose $\varepsilon_m = 10^{-16}$ and c_1, c_2 are both order 1. Estimate the order of magnitude of the best step size $h^\star$ and the best attainable error $E(h^\star)$ (order of magnitude only).

Q5. (**Moderate**, **Long Answer**) **[7 pts]**

Derive the central-difference approximation for $f'(x)$:

$$D_c(h) = \frac{f(x+h/2) - f(x-h/2)}{h}.$$

Using Taylor expansions about x, show that the leading truncation term is $\mathcal{O}(h^2)$.

Q6. (**Moderate**, **Long Answer**) **[7 pts]**

Let $p(x) = 5x^3 + 4x^2 + 3x + 2$.

(a) Compute $p'(x)$ analytically.

(b) Show that the central-difference formula $D_c(h)$ from Q5 yields $p'(x)$ *exactly* for all x (in exact arithmetic), regardless of $h \neq 0$. (Hint: expand $p(x \pm h/2)$ and cancel terms.)

(c) Explain why, in floating-point arithmetic, the result may still fail to be 100% precise for extremely small h.

Q7. (**Difficult**, **Long Answer**) **[12 pts]**

A higher-order derivative formula (built by cancellation) is:

$$D_4(h) = \frac{8f(x+h/4) + f(x-h/2) - 8f(x-h/4) - f(x+h/2)}{3h}.$$

(a) Using Taylor expansions about x, show that the $\mathcal{O}(h^2)$ truncation term cancels and the leading truncation error is $\mathcal{O}(h^4)$.

(b) Compared to $D_c(h)$, discuss when $D_4(h)$ is expected to be superior *in practice*, and when it may not be.

Q8. (**Moderate**, **Long Answer**) **[7 pts]**
Derive the standard central-difference approximation for the *second* derivative:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

(a) Show the truncation error order.

(b) Propose an error model incorporating a round-off term and discuss (qualitatively) how the optimal h should scale with ε_m.

Q9. (**Easy**, **Short Answer**) **[3 pts]**
Give a concise explanation (2–4 sentences) of the phrase: "compute the second derivative by calculating the first derivative twice." Then show the key algebraic step that turns a difference of first differences into a formula involving only $f(x+h), f(x), f(x-h)$.

Q10. (**Difficult**, **Long Answer**) **[11 pts]**
Adaptive stepping idea. Suppose you are estimating $f'(x)$ for a black-box f. Design an adaptive rule that updates step size h based on an estimate of:

- rounding error ε_R and
- truncation/approximation error ε_T.

Assume an update of the form

$$h_{\text{new}} = h \left(\frac{\varepsilon_R}{2\varepsilon_T} \right)^{1/3}.$$

Task: Provide an algorithmic description: (i) how you would estimate ε_T from two computations at different step sizes; (ii) how you would set/estimate ε_R; (iii) how you would update h and terminate. State at least one failure mode of this approach.

2 Numerical Integration (Q11–Q22)

1. (**Moderate**, **Short Answer**) **[6 pts]**
Write the composite trapezoidal rule for approximating $\int_a^b f(x)\,dx$ using N subintervals and step size $h = (b-a)/N$. State the global truncation error order (in h) for sufficiently smooth f.

2. (**Moderate**, **Long Answer**) **[7 pts]**
Compute a trapezoidal-rule approximation of

$$\int_0^{1.2} \left(x - x^2 + x^3 - x^4 + \frac{\sin(13x)}{13} \right) dx$$

using step size $h = 0.2$.

(a) list the grid points;

(b) write the weighted sum;

(c) compute the numerical value (calculator allowed).

Then briefly comment on the expected accuracy relative to using a much smaller h.

3. (**Moderate**, **Long Answer**) **[7 pts]**
Derive Simpson's rule on $[x, x+2h]$ by fitting a quadratic through three points $\{(x, f(x)), (x+h, f(x+h)), (x+2h, f(x+2h))\}$ and integrating that quadratic exactly.

4. (**Difficult**, **Long Answer**) **[11 pts]**
Using Taylor expansions, analyze Simpson's rule error on a single panel $[x, x+2h]$ and show that:

   (a) the leading neglected term involves $f^{(4)}(x)$ (or a nearby point);

   (b) the single-panel error is $\mathcal{O}(h^5)$;

   (c) for a fixed interval length $L = b - a$, the composite Simpson rule global truncation error is $\mathcal{O}(h^4)$.

5. (**Easy**, **Short Answer**) **[3 pts]**
Suppose composite Simpson uses step size $h = 10^{-3}$ over $[0, 1.2]$. Approximately how many function evaluations does it require? Compare this to a Gaussian quadrature method that uses a fixed $n = 21$ points over the same interval (in terms of evaluation count only).

6. (**Moderate**, **Long Answer**) **[7 pts]**
Two-point Gauss–Legendre quadrature on $[-1, 1]$ uses nodes $\pm 1/\sqrt{3}$ and equal weights.

   (a) Starting from the requirement that the rule be exact for $1, x, x^2, x^3$, set up the system of equations for the unknown nodes and weights.

   (b) Use symmetry to reduce the unknowns and solve the system.

   (c) Conclude that the rule integrates any cubic polynomial exactly on $[-1, 1]$.

7. (**Difficult**, **Long Answer**) **[12 pts]**
Derive the *three-point* Gauss-Legendre quadrature rule on $[-1, 1]$ by imposing exactness for monomials $1, x, x^2, x^3, x^4, x^5$.

   (a) Use symmetry to argue the node structure should be $x_2 = 0$ and $x_1 = -x_3$ with $w_1 = w_3$.

   (b) Solve for x_1, x_3, w_1, w_2, w_3.

   (c) Verify exactness for at least three monomials explicitly (show the computations).

8. (**Moderate**, **Long Answer**) **[7 pts]**
To apply Gauss–Legendre quadrature on an interval $[a, b]$, one maps it to $[-1, 1]$ via an affine transformation.

   (a) Derive the mapping $x = \frac{b-a}{2}t + \frac{a+b}{2}$ and the corresponding integral identity

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}t + \frac{a+b}{2}\right)\,dt.$$

   (b) Use the *two-point* Gauss-Legendre rule to approximate $\int_0^2 e^x\,dx$.

(c) Compare to the exact value $e^2 - 1$ (numerically) and report the absolute error.

9. (**Easy**, **Short Answer**) **[3 pts]**
An n-point Gauss-Legendre rule is exact for polynomials up to degree $2n - 1$. For $n = 5$, what is the highest degree integrated exactly? Then state whether degree-10 polynomials are guaranteed to be exact or not, and why.

10. (**Difficult**, **Long Answer**) **[11 pts]**
Integrating near singularities. Consider $\int_0^1 x^{-1/2}\,dx$.
    (a) Explain why uniform fixed-step rules (e.g., trapezoidal) can behave poorly near $x = 0$.
    (b) Propose two remedies: one based on a change of variables and one based on adaptivity/nonuniform meshing.
    (c) For the change-of-variables remedy, choose a substitution (e.g., $x = u^2$) and rewrite the integral into a form that is smooth at the left endpoint.

11. (**Easy**, **Short Answer**) **[3 pts]**
List two pros and two cons of "homemade code" versus "public/professional code" for numerical algorithms (bullet points are acceptable).

12. (**Moderate**, **Short Answer**) **[6 pts]**
A numerical derivative utility uses a central-difference style formula. Based on the idea that the error behaves like $\mathcal{O}(h^2) + \mathcal{O}(\varepsilon_m/h)$:
    (a) explain why the empirically best h is often around 10^{-5} to 10^{-6} in double precision;
    (b) explain why higher-order finite-difference stencils do *not* always lead to dramatic improvements in practice.

    (a) (**Easy**, **Short Answer**) **[4 pts]**
    Use the **2-point** Gauss–Legendre rule on $[-1, 1]$ to approximate

$$\int_{-1}^{1} \left(1 + 2x + 3x^2 + 4x^3\right)\,dx.$$

    State whether the result is *exact* and justify your claim using the "degree of exactness" property.

    (b) (**Moderate**, **Long Answer**) **[8 pts]**
    Use the **2-point** Gauss–Legendre rule on $[0, 2]$ to approximate

$$I = \int_0^2 e^x\,dx.$$

        (a) write the affine map $x(t)$ from $[-1, 1]$ to $[0, 2]$;
        (b) list the mapped nodes x_1, x_2;
        (c) write and evaluate the Gauss sum, then report the absolute error using the exact value $e^2 - 1$.

    (c) (**Moderate**, **Long Answer**) **[8 pts]**
    Use the **3-point** Gauss–Legendre rule on $[-1, 1]$ to approximate

$$I = \int_{-1}^{1} \frac{1}{1 + 25x^2}\,dx.$$

(a) Form the weighted sum $\sum_i w_i f(t_i)$.

(b) Briefly comment (1–3 sentences) on why oscillatory or sharply peaked integrands may require higher n or adaptivity.

3 Convexity and Optimization Foundations (Q23–Q30)

(a) (**Moderate**, **Long Answer**) **[7 pts]**
Convex sets.

- (a) State the definition of a convex set $C \subseteq \mathbb{R}^d$ in terms of line segments.
- (b) Prove that the intersection of two convex sets is convex. Your proof must explicitly use the definition.

(b) (**Moderate**, **Long Answer**) **[7 pts]**
Let $x_1 = (0,0)$, $x_2 = (1,0)$, $x_3 = (0,2)$ in $\mathbb{R}^2$.

- (a) Write the convex hull $\mathrm{co}(x_1, x_2, x_3)$ as a set of convex combinations.
- (b) Determine whether $z = (0.25, 0.5)$ lies in the convex hull by finding coefficients $\theta_i \geq 0$ summing to 1 (or proving none exist).
- (c) Give a geometric interpretation of your answer.

(c) (**Easy**, **Short Answer**) **[3 pts]**
Show that the halfspace $H = \{x \in \mathbb{R}^d : a^\top x \leq b\}$ is convex. Then answer: under what condition on b does H become a cone (i.e., closed under scaling by $\alpha > 0$)?

(d) (**Difficult**, **Long Answer**) **[11 pts]**
Convex functions and Jensen.

- (a) State the definition of a convex function $f : \mathbb{R}^d \to \mathbb{R}$.
- (b) Define midpoint convexity.
- (c) Prove (or outline a proof with clear steps) that if f is continuous and midpoint convex on an interval, then f is convex on that interval.

(e) (**Moderate**, **Long Answer**) **[7 pts]**
First-order characterization of convexity. Assume f is differentiable on a convex domain.

- (a) State the first-order condition: f is convex iff $f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle$ for all x, y in the domain.
- (b) Apply this condition to argue that $f(x) = \|x\|_2$ is convex on $\mathbb{R}^d$. (A full subgradient proof is not required; a clear argument suffices.)
- (c) Is $\sin(x)$ convex in $[0, \pi]$? Show if first order condition is voilated, some example will suffice.

(f) (**Moderate**, **Long Answer**) **[7 pts]**
Norms.

- (a) State the three norm axioms: definiteness, positive homogeneity, and triangle inequality.
- (b) Prove that any norm is a convex function (show the key inequality, not just a one-line claim).
- (c) Verify that $\|x\|_p = \left(\sum_i |x_i|^p\right)^{1/p}$ is a norm for $p \geq 1$ by checking the axioms (you may cite Minkowski for the triangle inequality if you clearly state it).

(g) (**Difficult**, **Long Answer**) **[11 pts]**
Dual norms and Hölder's inequality. Let $\|\cdot\|$ be a norm on $\mathbb{R}^d$ and define its dual norm

$$\|u\|_* = \sup\{u^\top x : \ \|x\| \le 1\}.$$

(a) Prove that $\|\cdot\|_*$ is a norm.
(b) Prove the generalized Hölder inequality $u^\top x \le \|u\|_* \, \|x\|$.
(c) Compute explicitly: the dual of $\|\cdot\|_1$ and the dual of $\|\cdot\|_\infty$.

(h) (**Difficult**, **Long Answer**) **[12 pts]**
Schur complement via partial minimization. Let $C \succ 0$ and consider the block matrix

$$Z = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \succeq 0.$$

Define the quadratic form $L(x,y) = \begin{pmatrix} x \\ y \end{pmatrix}^\top Z \begin{pmatrix} x \\ y \end{pmatrix}$.

(a) Expand $L(x,y)$ into $x^\top Ax + 2x^\top By + y^\top Cy$.
(b) Minimize $L(x,y)$ over y for fixed x by solving $\nabla_y L(x,y) = 0$.
(c) Substitute the minimizer $y^\star(x)$ back into L to show that the minimized value equals $x^\top(A - BC^{-1}B^\top)x$.
(d) Conclude that $A - BC^{-1}B^\top \succeq 0$.

(i) (**Easy**, **Short Answer**) **[4 pts]**
Write the gradient descent update rule and state (in one sentence) what information is needed at each iteration to compute $x^{(k+1)}$ from $x^{(k)}$.

(j) (**Moderate**, **Long Answer**) **[10 pts]**
Three explicit GD steps on a quadratic. Consider

$$f(x) = \frac{1}{2}x^\top Qx - b^\top x, \qquad Q = \begin{pmatrix} 4 & 1 \\ 1 & 3 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 2 \end{pmatrix}.$$

(a) Show that $\nabla f(x) = Qx - b$.
(b) Starting from $x^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and stepsize $\eta = 0.1$, compute $x^{(1)}, x^{(2)}, x^{(3)}$. You must show at least **three** explicit steps per iteration: compute gradient, multiply by η, update.
(c) Compute $f(x^{(0)}), f(x^{(1)}), f(x^{(2)}), f(x^{(3)})$ and comment on monotonic decrease (if any).

(k) (**Difficult**, **Long Answer**) **[13 pts]**
Three steps with backtracking line search (Armijo). Let $f(x) = \frac{1}{2}\|Ax - y\|_2^2$ with

$$A = \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}, \qquad y = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad x^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Use gradient descent with backtracking line search: start with trial stepsize $\eta = 1$, shrink by factor $\beta = 1/2$ until the Armijo condition

$$f(x - \eta\nabla f(x)) \le f(x) - c\,\eta\|\nabla f(x)\|_2^2$$

holds, with $c = 10^{-4}$.

(a) Derive $\nabla f(x) = A^\top (Ax - y)$.

(b) Perform **three iterations** producing $x^{(1)}, x^{(2)}, x^{(3)}$, showing your accepted stepsizes each time.

(c) Briefly explain why line search can help when a constant stepsize is unstable.