Assignment 2

Due in lecture on Oct. 31

Complete the following problems. There are three problems, each with multiple parts. The point value for each part is given with the problems below. For parts with multiple subparts, the point allocation between the subparts will be roughly uniform.

For each problem, your answer should include a clear, complete, and concise write-up documenting any mathematical developments or proofs required, any plots and explanations requested, a listing of any code necessary to complete the problem, and any screen output produced by running the code.

For problems requiring code, you may use Matlab or any language commonly used in scientific computing (e.g., Fortran, C, C++, etc.). For operations that you are not specifically asked to implement, you may use a library implementation if you choose.

Problem 1: Interpolation (30 points) In this problem, you will examine polynomial interpolation in 1-D.

1. (15 points) We saw in lecture that polynomial interpolation with n uniformly spaced points gives the following error bound:

$$\|e_{n-1}\|_\infty \le \frac{Mh^n}{4n},$$

   where $M \le \|f^{(n)}\|_\infty$. Use this result to develop a bound for the error in a polynomial interpolant of $\sin(x)$ on the interval $[0, \pi/2]$ constructed using uniformly spaced points. Does the resulting bound converge or diverge as n grows? Assess your result by computing the polynomial interpolant for $n = 2$ (i.e., linear polynomials) through $n = 10$ (i.e., 9th order polynomials) and approximating the ∞-norm of the error. You may write your own polynomial interpolation or use a library routine.

2. (15 points) Consider cubic spline interpolation on the interval $[a, c]$ split into two subintervals $[a, b]$, $[b, c]$ (where $a < b < c$).

   (a) With two subintervals and cubic polynomials on each subinterval, we have 8 degrees of freedom that define the piecewise cubic splines. Specifically, using a monomial basis, we have

$$p_L(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3, \quad a \le x \le b$$
$$p_R(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, \quad b \le x \le c.$$

   Given the values $f(a)$, $f(b)$, and $f(c)$ of the function we wish to interpolate, write out the system of 8 equations that one would solve to determine the values α_i and β_i. Use "natural" end conditions—i.e., $p''_L(x = a) = 0$ and $p''_R(x = c) = 0$.

(b) Solve the system you developed above for the following inputs: $a = -1$, $b = 0$, $c = 1$, $f(a) = -1$, $f(b) = 0$, $f(c) = 1$. To visually assess whether your result satisfies the desired conditions (i.e., that it matches the data, has the desired number of continuous derivatives and the requested behavior at the boundaries), generate a plot of the interpolant as well as its first and second derivatives.

(c) Note that the above data is consistent with $f(x) = x^3$. However, the interpolant from part 2 is not this function. Explain why and show how the equations you developed should be modified to ensure that if the function generating the data is cubic, the cubic spline will exactly reproduce it. *Hint: You will need more information from the function to accomplish this. Think about the end conditions.*

Problem 2: 1-D Quadrature and Error Estimation (40 points) In this problem, you will explore the errors in the some of the 1-D quadrature rules we introduced in class.

1. (10 points) In class, we demonstrated that

$$I(f) = \int_a^b f dx = f(\bar{x})(b-a) + \frac{1}{24} f''(\bar{x})(b-a)^3 + O((b-a)^5),$$

   where $\bar{x} = (b+a)/2$. This shows that, for a single interval, the midpoint rule is third-order accurate. Perform a similar Taylor series analysis for the trapezoidal rule. *Hint: Start by writing Taylor series expansions for $f(a)$ and $f(b)$ about the midpoint $\bar{x}$.*

   Based on this analysis, what is the order of accuracy of the trapezoidal rule for a single interval? Which rule (midpoint or trapezoidal) do you expect to be more accurate when the interval length is small (i.e., such that $(b-a)^5 \ll (b-a)^3$)?

   Given your results, formulate a way to estimate the leading order error (for either the trapezoidal or midpoint rule) based on the difference between the results given by the two rules.

2. (10 points) Using a weighted sum of the trapezoidal and midpoint rules and your Taylor series analysis from part 1, show that Simpson's rule applied to a single interval is 5th order.

3. (10 points) Use midpoint, trapezoidal, and Simpson's rule in composite form (i.e., subdivide the integration domain into multiple subintervals and apply midpoint, trapezoidal, and Simpson to each subinterval) on a uniform mesh to evaluate two functions of your choosing that you can integrate analytically. You may use library routines or code your own implementation of the quadrature schemes. If you choose a polynomial as one of your functions, make sure it is degree 4 or higher such that none of the rules gives the exact result.

   Use your analytic results to compute the integration error for each approach as you increase the number of subintervals (i.e., as you decrease the subinterval size h while keeping the total interval length fixed). Present your results in a log-log plot such that the order of accuracy for each method is easily apparent.

   Are the results consistent with your error analysis? Explain.

4. (10 points) Use Richardson extrapolation with your two finest Simpson's rule results from part 3 to produce a more accurate estimate.

Problem 3: Finite Difference Derivatives (30 points) In this problem, you will investigate some typical finite difference schemes.

1. (15 points) In this problem, you will perform a modified wavenumber analysis of two 4th order approximations of the first derivative. Throughout the problem, the mesh is taken to be uniform.

   The two approximations we will analyze are the 4th order central difference given by

   $$f'_j = \frac{-f_{j+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + O(h^4).$$

   and a 4th order Padé scheme defined by

   $$f'_{j+1} + 4f'_j + f'_{j-1} = \frac{3(f_{j+1} - f_{j-1})}{h} + O(h^4).$$

   Derive the modified wavenumber $\tilde{k}$ associated with each of these schemes. *Hint: For the 4th order central scheme, proceed exactly as we did for the 2nd order central scheme in class. For the Padé scheme, assume that $f'_j = i\tilde{k}\exp(ikx_j)$ to evaluate the left-hand side. Treat the right-hand side the same as we did in class, and solve for $\tilde{k}$.*

   Show both of your results as well as the result for the 2nd order scheme derived in the class notes on a $\tilde{k}h$ versus kh plot. Comment on your results, particularly at high wavenumber.

2. (15 points) Consider the following function:

   $$f(x) = 1 - \frac{1}{6}x^2 - \frac{5}{6}x^{32}, \quad x \in [-1, 1].$$

   Using the centered second-order scheme for the first derivative, compute f' on a uniform grid. Plot the convergence of the maximum absolute value of the error in this approximation on a log-log scale versus the grid spacing h.

   Now, consider the mapping

   $$x = \frac{\sin\left(\alpha\frac{\pi}{2}\xi\right)}{\sin\left(\alpha\frac{\pi}{2}\right)}$$

   for $\xi \in [-1, 1]$ with $\alpha = 0.8$. Generate a uniform mesh of the ξ coordinate. Use this mesh and the mapping above to compute f' using a centered second-order scheme (applied in ξ space). Plot the maximum absolute value of the error versus h on the same log-log plot as your previous result.