Fall 2022: Numerical Analysis
Assignment 6 (due Dec 15, 2022 at 11:59pm ET)

2 extra credit points will again be given for generally cleanly written and reasonably well-organized homework. This includes cleanly plotted and labeled figures (see also rules on the first assignment).

1. **[Hermite interpolation, 3pts]** Let $x_0 = 0, x_1 = 1, x_2 = 2$. Recall that the Hermite interpolant of a function f at the points x_0, x_1, x_2 has the form

$$p(x) = \sum_{j=0}^{2} H_j(x) f(x_j) + \sum_{j=0}^{2} K_j(x) f'(x_j).$$

   (a) Show that the polynomial $H_1(x)$ in this representation is given by

$$x^4 - 4x^3 + 4x^2.$$

   (b) Verify that the polynomial $K_1(x)$ in this representation is

$$x^5 - 5x^4 + 8x^3 - 4x^2.$$

   (c) Sketch $H_2(x)$ and $K_2(x)$ in the same graph without computing their exact form explicitly.

2. **[Interpolating polynomials, 1+1+2pts]**

   (a) Write down the interpolating polynomial in Lagrange form of degree 1 for the function $f(x) = x^3$ using the points $x_0 = 0$ and $x_1 = a$.

   (b) Theorem 6.2 in the text states that for $x \in [0, a]$, there exists a $\xi = \xi(x) \in (0, a)$ such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j).$$

   Here, n is the degree of the interpolating polynomial p_n. Verify the above formula, by direct calculation, for the function and interpolating polynomial from part (a). Show that in this case, ξ is unique and has the value $\xi = \frac{1}{3}(x + a)$.

   (c) Repeat parts (a) and (b) for the function $f(x) = (2x - a)^4$. This time, show that there are two possible values for ξ, and give their values.

3. **Simpson's rule and interpolation [3pts]**

   (a) Recall the error estimate for the Simpson's rule given by

$$|E_2(f)| \leq \frac{(b-a)^5}{2880} M_4,$$

   where $M_4 = \max_{x \in [a,b]} |f^{(iv)}(x)|$. Here, $f^{(iv)}$ denotes the 4-th derivative of f. Use this estimate to explain which functions f are integrated exactly by the Simpson's rule.

   (b) Let $f(x) = \frac{1}{4}x^4 + \sin(x)$. According to the error estimate, what is the maximal error you will make when integrating f over $[0, \pi]$? You do not need to calculate the approximate integral.

(c) Consider the interpolation nodes $x_0 = 0, x_1 = 1, x_2 = 2$. Sketch the Lagrange interpolation polynomial $L_0(x)$, and the Hermite interpolation polynomials $H_1(x)$ and $K_2(x)$. Note that you do not need to compute these polynomials, just sketch them based on the conditions they satisfy at their node points.

4. **[Composite integration, 2+2+2pt]** Write a code[1] to approximate integrals of the form

$$I(f) = \int_a^b f(t)\,dt$$

using the trapezoidal rule or Simpson's rule on the sub-intervals $[x_{i-1}, x_i]$, $i = 1, \dots, m$, where $x_i = a + ih$, $i = 0, \dots, m$ with $h = (b-a)/m$.[2]

(a) Hand in listings of your codes, and use them to approximate the integral

$$\int_{0.1}^1 \sqrt{x}\,dx.$$

Compare the numerical errors $\mathcal{E}$ for different m (e.g., $m = 10, 20, 40, 80, \dots$) and plot the quadrature errors versus m in a double-logarithmic plot. The exact value of the integral is $\frac{2}{3} - \frac{1}{15\sqrt{10}}$.

(b) To numerically study how the errors $\mathcal{E}$ decrease with m, we assume that the errors behaves like Cm^κ, with to-be-determined $C, \kappa \in \mathbb{R}$. Applying the logarithm to $\mathcal{E} = Cm^\kappa$ results in

$$\log(\mathcal{E}) = D + \kappa \log(m), \tag{1}$$

where $D = \log(C)$. Use the values for m and $\log(\mathcal{E})$ you computed in (a) to find the best-fitting values for D and κ in (1) by solving a least squares problem. Compare your findings for κ with the theoretical estimates for the composite trapezoidal rule.[3]

(c) Repeat steps (a) and (b) using $a = 0$ instead of $a = 0.1$ as lower integration bound. Can the theoretical estimates still be applied and why/why not?

5. **[An alternative composite Integration rule, 1+1+2pts]** Consider the composite *midpoint rule* for approximating an integral

$$\int_a^b f(x)dx \approx h \sum_{i=1}^n f\left(\frac{x_i + x_{i-1}}{2}\right)$$

with $h = (b-a)/n$ and $x_i = a + ih$, $i = 0, 1, \dots, n$.

(a) Draw a graph that shows geometrically what area is being computed by this formula.

(b) Show that this formula is exact if f is either constant or linear in each subinterval.

[1] Ideally, you write a function `trapez(f,a,b,m)`, where f is a function handle (see `http://www.mathworks.com/help/matlab/matlab_prog/creating-a-function-handle.html` if you are not familiar with that concept) or f is the vector $(f(x_0), \dots, f(x_m))$.

[2] For composite rules, see Definitions 7.1 and 7.2 in the book.

[3] Compare with (7.16) in the book. You can ignore the constants, just compare κ, the exponent of m, with the theoretical results.

(c) Assuming that $f \in C^2([a,b])$, show that the midpoint rule is second-order accurate. That is, the error is less than or equal to a constant times h^2. To do this, you will first need to show that the error in each subinterval is order h^3. To see this, expand f in a Taylor series about the midpoint $x_{i+1/2} = \frac{1}{2}(x_i + x_{i-1})$ of the subinterval (with exact remainder). By integating each term, show that the difference between the true value $\int_{x_{i-1}}^{x_i} f(x)dx$ and the approximation $hf(x_{i+1/2})$ is of order h^3. Finally, combine the results from all subintervals to show that the total error is of order h^2.

6. **[Newton-Cotes vs. Gauss Quadrature, 2+2+2+1pt]** We discussed two methods to integrate functions numerically, namely the Newton-Cotes formulas and Gauss quadrature.

   (a) Recall that we calculated the first three orthogonal polynimals with respect to $w \equiv 1$ on $(0,1)$ in class to be $\{p_0, p_1, p_2\} = \{1, x-1/2, x^2-x+1/6\}$. Calculate $p_3(x)$ using the ansatz $p_3(x) = x^3 - a_2p_2(x) - a_1p_1(x) - a_0p_0(x)$, with appropriately computed $a_2, a_1, a_0 \in \mathbb{R}$.

   (b) Derive the Gaussian Quadrature formula for $n = 2$, i.e., calculate both the quadrature points x_0, x_1, x_2 (these are the roots of p_3 and the corresponding weights W_0, W_1, W_2.[4]

   (c) Now we want to compare Gaussian quadrature derived in (b) with the Simpson's Rule. Use both methods to numerically find

   $$I_k = \int_0^1 x^k + x\,dx, \qquad \text{for} \quad k = 1, \ldots, 7.$$

   Plot the errors arising in each method as a function of k. Note that to find the error, you will need to calculate the exact values for I_k (by hand).

   (d) Explain your findings using the results on the exact integration for polynomials up to certain degrees discussed in class.

7. **[Orthogonal polynomials on $[0,\infty)$, 2+2+2pt extra credit]**

   (a) Find orthogonal polynomials l_0, l_1, l_2, l_3 for the unbounded interval $[0,\infty)$ with the weight function $\omega(x) = \exp(-x)$.[5] Plot these polynomials (they are called *Laguerre polynomials*).

   (b) As these are orthogonal polynomials, they correspond to a quadrature rule for weighted integrals on $[0,\infty)$. The resulting quadrature points and weight are given in Table 1. Verify that for $n = 2$, $n = 3$, the quadrature nodes x_i are the roots of the polynomials $l_2(x), l_3(x)$ (up to round-off).

   (c) Use the quadrature rules from Table 1 to approximate the integrals

   $$\int_0^\infty \exp(-x)\exp(-x)\,dx \quad \text{and} \quad \int_0^\infty \exp(-x^2)\,dx.$$

   Note that, to take into account the weight $\omega(x) = \exp(-x)$, for the first integral $f(x) = \exp(-x)$ and for the second $f(x) = \exp(-x^2 + x)$. Report the errors for $n = 2, 3, 4$ using that the exact values for the integrals are $1/2$ and $\sqrt{\pi}/2$.

[4] See equation (10.7) in the book.

[5] Feel free to look up the values for the indefinite integrals $\int_0^\infty \exp(-t)t^k\,dx$ $(k = 0, 1, 2, 3)$—I use Wolfram Alpha for looking up things like that: http://www.wolframalpha.com/.

Table 1: Gauss quadrature points and weights for quadrature on $[0, \infty)$.

n	x_i	W_i
2	0.585786	0.853553
	3.41421	0.146447
3	0.415775	0.711093
	2.29428	0.278518
	6.28995	0.0103893
4	0.322548	0.603154
	1.74576	0.357419
	4.53662	0.0388879
	9.39507	0.000539295