Fall 2018: Numerical Analysis Assignment 6 (due December 6, 2018)

2 extra credit points will again be given for cleanly plotted and labeled figures (see also rules on the first assignment).

1. [Hermite interpolation] Let $x_0 = 0, x_1 = 1, x_2 = 2$. Recall that the Hermite interpolation 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.
- [Composite trapezoidal and Simpson sum, 4+2pt] Write codes¹ to approximate integrals of the form

$$I(f) = \int_{a}^{b} f(t) \, dt$$

using the trapezoidal and Simpson's rule on the sub-intervals $[x_{i-1}, x_i]$, i = 1, ..., m, where $x_i = a + ih$, i = 0, ..., 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 both quadrature rules (the exact value of the integral is $\frac{2}{3} - \frac{1}{15\sqrt{10}}$). Try different m (e.g., $m = 10, 20, 40, 80, \ldots$) and plot the quadrature errors versus m in a double-logarithmic plot.

¹Ideally, you write functions trapez(f,a,b,m) and simpson(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 $(f(x_0), \ldots, f(x_m))$.

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

(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 and Simpson's rules.³

3. [Best 2-norm approximation, 2pt] The upper row in the below figure shows a function f together with a polynomial approximation. For three plots, the optimal best 2-norm fit for three different weights w(x) is used, and one is the result of an Lagrange interpolation. Match the approximations in the upper row with the information (weight functions or interpolation points) in the lower row.



- [Orthogonal polynomials, 2+2pt] Remember that a function f is called *even* if f(-x) = f(x) and odd if f(-x) = -f(x) for all x in its domain. Let w be an even weight function on the interval (-a, a) and {φ₀, φ₁, ..., φ_n} be a system of orthogonal polynomials on (-a, a) with respect to w, constructed from the monomial basis 1, x, x², ... using Gram-Schmidt-Orthogonalization.
 - (a) Show that, if j is even, then φ_j is an even function and if j is odd, then φ_j is an odd function.

³Compare with (7.16) and (7.18) in the book. You can ignore the constants, just compare κ , the exponent of m, with the theoretical results.

- (b) Let $f : [-a, a] \to \mathbb{R}$ and $p_n(x) = \gamma_0 \varphi_0(x) + \ldots + \gamma_n \varphi_n(x)$ its best polynomial approximation of degree n with respect to the weighted 2-norm. Show that if f is an even function, then all the odd coefficients γ_{2j-1} are zero and if f is an odd function, then all the even coefficients γ_{2j} are zero.
- 5. **[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 $\{\varphi_0, \varphi_1, \varphi_2\} = \{1, x - 1/2, x^2 - x + 1/6\}$. Calculate $\varphi_3(x)$ using the ansatz $\varphi_3(x) = x^3 - a_2\varphi_2(x) - a_1\varphi_1(x) - a_0\varphi_0(x)$, 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 φ_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

$$I_k = \int_0^1 x^k \, dx, \qquad \text{for} \quad k = 0, \dots, 7.$$

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.

6. [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,∞). 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 l₂(x), l₃(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 $\sqrt{\pi}/2$.

⁴See equation (10.7) in the book.

⁵Feel 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/.

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

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