PHYS 581 Assignment 3

100 points total

Due Monday, March 3 at 11:59pm

1. (10 points) Using Lagrange basis polynomials defined on an evenly spaced grid (and Mathematica), derive the n-point integration formulas for $2 \leq n \leq 10$ following the procedure in Eqs. (1.45)-(1.49) in the notes. Verify that these match the trapezoidal and Simpson's rules for small n.

2. (90 points) All questions in this problem are focused on numerically solving for the value of the integrals

$$I_{jk} = \int_{-\infty}^{\infty} e^{-x^2} H_j(x) H_k(x), \quad 0 \leq j, k \leq 10,$$

where $H_j(x)$ are 'physicist' Hermite polynomials (see the wikipedia entry about different versions of Hermite polynomials) and the *weight function* is e^{-x^2}. The Hermite polynomials are defined by the recurrence relation

$$H_{j+1}(x) = 2xH_j(x) - 2jH_{j-1}(x),$$

subject to $H_{-1}(x) = 0$ and $H_0(x) = 1$. In Mathematica, these are the built-in functions `HermiteH[j,x]`. Tabulate the exact values of these integrals obtained in Mathematica for your reference.

   (a) (10 points) Because of the weight function, the integral converges quickly as $|x|$ increases when j, k are not too large, i.e. when $0 \leq j, k \leq 10$. Using C, determine the value of $x_{\max}$ for the integral, where for $|x| > x_{\max}$ the integrand is smaller than machine precision. [Note: the value of $x_{\max}$ will depend on j, k].

   (b) (20 points) Again in C, obtain the integrals using m evenly spaced gridpoints in the interval $-x_{\max} \leq x \leq x_{\max}$ obtained above, and the n-point integration rules obtained in question 1, for $n \ll m$. How large do you have to make m to ensure convergence to the exact value? Is there any advantage to using larger-n rules?

   (c) (60 points) Next perform the integral using Gaussian quadrature, based on both Hermite and Chebyshev polynomials. Because Chebyshev polynomials are only defined on $-1 \leq x \leq 1$, you will need to rescale your coordinates when using this quadrature.

      i. (10 points) Using Mathematica, obtain the roots by numerically solving for the zeroes of the degree-m polynomials `HermiteH` and `ChebyshevT`, for some value of m large enough to well-represent the integrand.

      ii. (10 points) Using Mathematica, obtain the Gaussian quadrature weights using any of Eqs. (1.83), (1.90), or (1.97) in the course notes, for both Hermite and Chebyshev polynomials. The Chebyshev weights should turn out to be constant, $w_j = \pi/m$, as shown in the course notes, pp. 21-23.

      iii. (20 points) In C, using the roots and weights determined above, obtain the values of the integral via Gaussian quadrature. How well do the results match the exact values? How large does m need to become in each case to obtain the value of the integral to six decimal places?

      iv. (20 points) Using Mathematica, obtain the roots and weights for some arbitrary m for both the Hermite and Chebyshev cases, by diagonalizing the $\mathcal{J}$ matrix, Eq. (1.100) in the notes. Be sure to check that the results match the numerical solutions for the zeroes of the mth-degree polynomials used in the calculations above.