Assignment-7

PHY617/473-Computational Physics
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Question 1. **Quantum uncertainty in the harmonic oscillator** In units where all the constants are 1, the wavefunction of the nth energy level of the one-dimensional quantum harmonic oscillator—i.e., a spinless point particle in a quadratic potential well—is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2} H_n(x),$$

for $n = 0 \ldots \infty$, where $H_n(x)$ is the nth Hermite polynomial. Hermite polynomials satisfy a relation somewhat similar to that for the Fibonacci numbers, although more complex:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

The first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$.

1. Write a user-defined function `H(n,x)` that calculates $H_n(x)$ for given x and any integer $n \geq 0$. Use your function to make a plot that shows the harmonic oscillator wavefunctions for $n = 0$, 1, 2, and 3, all on the same graph, in the range $x = -4$ to $x = 4$. Hint: There is a function `factorial` in the `math` package that calculates the factorial of an integer.
2. Make a separate plot of the wavefunction for $n = 30$ from $x = -10$ to $x = 10$. Hint: If your program takes too long to run in this case, then you're doing the calculation wrong—the program should take only a second or so to run.
3. The quantum uncertainty of a particle in the nth level of a quantum harmonic oscillator can be quantified by its root-mean-square position $\sqrt{< x^2 >}$, where

$$< x^2 >= \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \, dx.$$

Write a program that evaluates this integral using Gaussian quadrature on 100 points and then calculates the uncertainty (i.e., the root-mean-square position of the particle) for a given value of n. Use your program to calculate the uncertainty for $n = 5$. You should get an answer in the vicinity of $\sqrt{< x^2 >} = 2.3$.

Question 2 Evalute the integral using Gaussian quadrature

$$\int_{-1}^{1} \int_{-1}^{1} \cos\frac{\pi x}{2} \cos\frac{\pi y}{2} dxdy$$

Question 3. Create a user-defined function `f(x)` that returns the value $1 + \frac{1}{2}\tanh 2x$, then use a central difference to calculate the derivative of the function in the range $-2 \leq x \leq 2$. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots.

Question 4. Even when we can find the value of $f(x)$ for any value of x the forward difference can still be more accurate than the central difference for sufficiently large h. For what values of h will the approximation error on the forward difference be smaller than on the central difference?