Hw 5

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Learned the computation and plotting of the error function of an integral using Trapezoidal integration and Gaussian quadrature and how to calculate the quantum uncertainty in the harmonic oscillator

1. INTRODUCTION

For this homework assignment, I practiced ways to evaluate integrals, as well as to how to compare their error as a function of N. One of this ways in to use the Trapezoidal rule, which was talked about in the last assignment. For this assignment specifically, the Gaussian quadrature method will be explained as well as to the calculation of both the trapezoidal integration and Gaussian quadrature error.

Gaussian quadrature is a numerical integration method that uses weighted sum of function values at specific points to approximate the integral of a function over a given interval. The correct rule for mapping the points to a general domain that runs from x=a to x=b is:

$$x'_{\mathrm{k}} = \frac{1}{2}(b-a)x_{\mathrm{k}} + \frac{1}{2}(b+a) \tag{1}$$

As for the weights, they don't change if the sample points is sliding up and down the x line, but if the width of the integration domain changes then the value of the integral will increase or decrease by a corresponding factor, which means the weights have to be re-scaled using

$$w'_{\mathrm{k}} = \frac{1}{2}(b-a)w_{\mathrm{k}} \tag{2}$$

After calculating the re-scaled positions and weights then the integral itself is given by

$$\int_a^b f(x)\,dx \;\approx \sum_{k=1}^{n} w'_{\mathrm{k}} f(x'_{\mathrm{k}}) \tag{3}$$

The basic idea behind Gaussian quadrature is to approximate the integral of a function f(x) over an interval [a, b] as a weighted sum of N points so that the integration rule is exact for all polynomial integrands up to and including polynomials of degree $2N-1$. To get an integration rule accurate up to the highest possible degree of $2N-1$, the sample point x_{k} should be chosen to coincide with the zeros of the Nth Legendre Polynomial $P_{\mathrm{N}}(x)$, if necessary re-scaled to the window of integration using Eq.(1), and the corresponding weights $w_{\mathbf{k}}$ are

$$w_{\mathrm{k}} - \left[\frac{2}{(1-x^2)}\left(\frac{dP_{\mathrm{N}}}{dx}\right)^{-2}\right] \tag{4}$$

To use the method Gaussian quadrature, given the values for x_{k} and w_{k} for a chosen N, all there is to do is to re-scale them if necessary using Eq. (1) and Eq(2) and then perform the sum in Eq. (3)

The error of Gaussian quadrature depends on the smoothness of the function f(x) and the number of points used in the approximation. As mentioned earlier, Gaussian quadrature is exact for polynomials of degree up to 2n-1, which means that for a given number of points, the error decreases as the function being integrated becomes smoother.

I also learned about the quantum uncertainty in the harmonic oscillator. For this exercise I learned that in units where all the constants are 1, the wavefunction of the nth energy level of the two-dimensional quantum harmonic oscillator, which is a spinless point particle in a quadratic potential well and is given by

$$\psi_{\mathrm{n}}(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{\frac{-x^2}{2}} H_{\mathrm{n}}(x) \tag{5}$$

for $n = 0...\infty$, where $H_{\mathrm{n}}(x)$ is the nth Hermite polynomial. Hermite polynomials satisfy a relation somewhat similar to that for the Fibonacci numbers but more complex:

$$H_{\mathrm{n+1}}(x) = 2xH_{\mathrm{n}}(x) - 2nH_{\mathrm{n-1}}(x) \tag{6}$$

Which I can rewrite to isolate H_{n}

$$H_{\mathrm{n}}(x) = \frac{(H_{\mathrm{n+1}}(x) + 2nH_{\mathrm{n-1}}(x))}{2x} \tag{7}$$

Next, I used the recurrence relation again to substitute for $H_{\mathrm{n-1}}(x)$

$$H_{\mathrm{n}}(x) = \frac{H_{\mathrm{n+1}}(x) + 2n(H_{\mathrm{n}}(x) - 2xH_{\mathrm{n-1}}(x))}{2x} \tag{8}$$

Once I simplify, I get

$$2xH_{\mathrm{n}}(x) = H_{\mathrm{n+1}}(x) + 2nH_{\mathrm{n}}(x) - 4x(n-1)H_{\mathrm{n-1}}(x) \tag{9}$$

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Finally, after rearranging the equation, I get

$$H_{\rm n}(x) = 2xH_{\rm n-1}(x) - 2(n-1)H_{\rm n-2}(x) \tag{10}$$

Which I will use in exercise 5.13

I also learned that the quantum uncertainty in the position of a particle in the nth level of a harmonic oscillator can be quantified by its root-to-mean-square position $\sqrt{\langle x^2 \rangle}$, where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_{\rm n}(x)|^2 \, dx \tag{11}$$

2. EXERCISE 5.3 CONTINUATION

For this exercise, using the same integral as last assignment:

$$E(x) = \int_0^x e^{-t^2} \, dt \tag{12}$$

I had to write a program to calculate the integral $E(x)$ for values of x from 0 to 3 in steps of 01, using the trapezoidal rule, and the Gaussian quadrature , and then make a graph of the error of the trapezoidal integration and Gaussian quadrature as a function of N. I started by defining the function to integrate (e^{-t^2}). I then defined the trapezoidal integration the same way I did in the last assignment. Then I defined the Gaussian quadrature, where I use "fixed-quad" a function from scipy.integrate to numerically integrate the integral from 0 to x using Gaussian quadrature with n=5, then multiply the result by the square root of π to get the value of E(x). Next, I generated a sequence of values from 0 to 3 with a step of 0.1 for both methods, which I then use to calculate E(x) using both the trapezoidal rule and Gaussian quadrature. Finally I find the absolute error of each method and plot them as a function of N

3. EXERCISE 5.13

For part a) for this exercise I wrote a user-defined function H(n, x) by using the first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$ and Eq. (10) seen in the introduction. To do this, I created an if statement that returns 1 if n=0, it returns 2x if n=1, or if n is neither 0 nor 1, the function initializes the variables "Hn-minus-2" to 1 and "H-minus-1" to 2x. I then created a for loop that iterates i=2 to n. For each value of "i", the function calculates the value of Hn(x) using the Eq. (10), and once the loop is completed it returns the value of Hn(x). To make the plot that shows the harmonic oscillator wavefunctions for n= 0, 1, 2 and 3 all on the same graph, I incorporated the range of x=-4 to x=4 by creating an array of 1000 equally spaces points between -4 and 4, I then put the labels and and title. To make the actual plot I created a for loop that iterates over the values of n from 0 to 3 and calculates the corresponding values of Hn(x) for each value of x in the range. It then plots the resulting wavefunctions on the same graph.

For part b) I did the same thing than part a, except that for the array I did the range between -10 to 10, and since I only needed a plot for the wavefunction for n=30, instead of doing a for loop for the values of n from 0 to 3, I just wrote a line that would calculate the corresponding value of H30(x), and then plot it

For part c) I defined the function that returns the value of the wave function ψ .I then defined another function that returns the integrad for the integral of $x^2|\psi_{\rm n}(x)|^2$ from $-\infty$ to ∞ since the Gaussian quadrature is only available for finite limits. I then created another function that will evaluate $x^2|\psi_{\rm n}(x)|^2$ using Gaussian quadrature with 100 points. Next, I created an uncertainty function that calculates the uncertainty of a particle in the harmonic oscillator potential for a given value of n. This uncertainty is calculated as the square root of the difference between the expectation value of x^2 and the square of the expectation value of x. Finally I calculated the uncertainty for n=5. by used the first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$.

4. RESULTS

For exercise 5.3 continuation, I got the following graph:

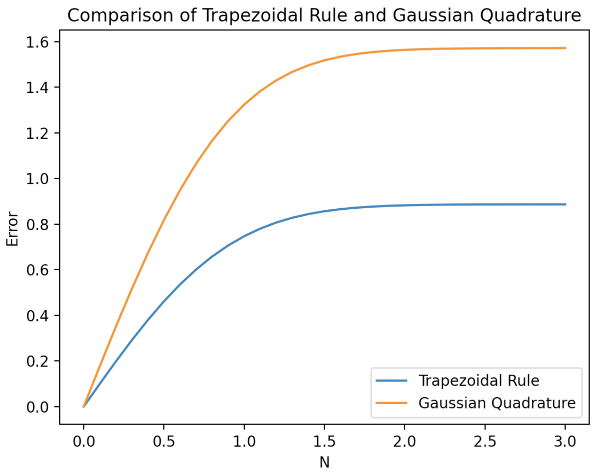

FIG. 1: Graph showing the Error of the Trapezoidal integration and Gaussian quadrature as a function of N for x values from 0 to 3 in steps of 0.1

For exercise 5.13, I got the following two graphs
For part a)

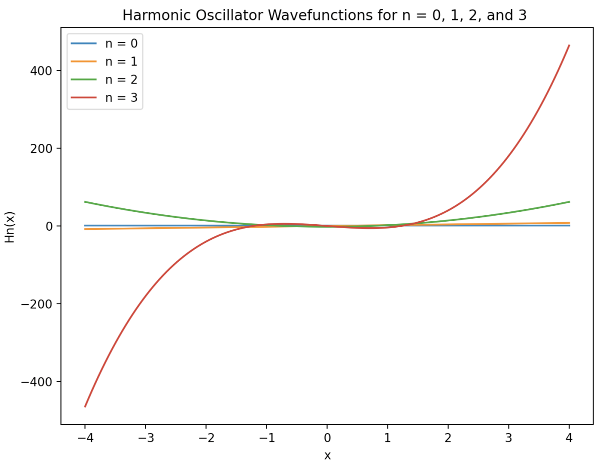

FIG. 2: Graph showing the harmonic oscillator wavefunctions for n = 0, 1, 2, and 3 in the range x =-4 to x=4

For part b)

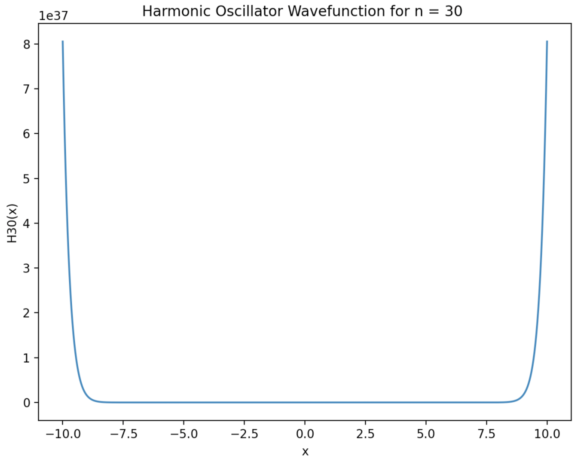

FIG. 3: Graph showing the harmonic oscillator wavefunction for n = 30 in the range x =-10 to x=10

5. CONCLUSION

Survey Questions For this assignment, it took me a long time mainly because I got ill and I found that exercise 5.13 was pretty hard and time consuming. I had some trouble on part c) since it kept saying that Gaussian quadrature is only available for finite limits, and I needed infinite limits. Which I then went back to the book and read some more, and I learned that when having infinite limits, we could use $x = tan(z)$. I feel like I learned a lot on this assignment, on both exercise, mainly seeing the both the trapezoidal and Gaussian quadrature curves on the plot for exercise 5.3 continuation, made me realizes the big difference they have, and now for future integration I will definitely use Gaussian quadrature. Once again, as I write more in overleaf, I get to learn more ways to use write symbols, and complex equations. Both programs were interesting to me, but I liked exercise 5.3 continuation since I could visibly see the difference between the two methods in the graph. Oh and I like flow charts better now. .