# Gauss-Hermite

SGTB Khalsa College, University of Delhi

Preetpal Singh(2020PHY1140)(20068567043)

Ankur Kumar(2020PHY1113)(20068567010)

Unique Paper Code: 32221401

Paper Title: Mathematical Physics III

Submitted on: February 8, 2022

B.Sc(H) Physics Sem IV

Submitted to: Dr. Mamta

# ${\bf Contents}$

1	Theory	i
2	Algorithm	iii
3	Programming	iii
4	Discussion	v

# 1 Theory

# Hermite Gauss Quadrature method for Integration

Hermite-Gauss quadrature is an extension of Gaussian quadrature over the interval  $(-\infty, \infty)$ . It fits all polynomials of degree 2m-1 exactly. This method approximates the value of integrals of the following kind:

$$\int_{-\infty}^{+\infty} e^{-x^2} g(x) dx \approx \sum_{i=1}^{n} w_i g(x_i)$$

here  $x_i$  is the *i*-th root of Hermite polynomial  $H_n(x)$  and the weight  $w_i$  is,

$$w_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 \left[ H_{n-1} \left( x_i \right) \right]^2}$$

# Hermite differential equation

The Hermite polynomials are solutions of second-order linear Hermite differential equation:

$$y'' - 2xy' + 2ky = 0$$

where constant k can be any real number.

The Hermite polynomials are defined by given formula,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left( e^{-x^2} \right)$$

The first five Hermite polynomials are denoted by  $H_0, H_1, H_2, H_3, H_4$ , which are following,

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x$$

$$H_4(x) = 16x^4 - 48x^2 + 12$$

## Recursion Formulae for Hermite Polynomials

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$
$$H'_n(x) = 2nH_{n-1}(x)$$

## Orthogonality properties for Hermite Polynomials

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 0 \quad \text{when } m \neq n$$

$$\int_{-\infty}^{\infty} e^{-x^2} [H_n(x)]^2 dx = 2^n n! \sqrt{\pi} \quad \text{when } m = n$$

## 2-point Quadrature Formula for Gauss Hermite Polynomials

As we know for N point method,

$$I_n = \sum_{i=1}^{N} w_i f(x_i)$$

$$I_n = \int_{-\infty}^{\infty} g(x) e^{-x^2} dx = \omega_0 g(x_0) + \omega_1 g(x_1) + \dots + \omega_n g(x_n)$$

For 2 point formula,

$$I(g) = \int_{-\infty}^{\infty} g(x)e^{-x^2}dx = \omega_0 g(x_0) + \omega_1 g(x_1) = I_2(g)$$

As there are 4 unknowns  $x_0, x_1, \omega_0, \omega_1$  so approximating these with 4 polynomials of degree less than or equal to 3.

$$g(x) = 1, x, x^2, x^3$$

$$g(x) = 1 \quad \int_{-\infty}^{\infty} g(x)e^{-x^2}dx = \int_{-\infty}^{\infty} e^{-x^2}dx = \omega_0 g(x_0) + \omega_1 g(x_1) = \omega_0 + \omega_1 = \sqrt{\pi}$$
$$g(x) = x \quad \omega_0 x_1 + \omega_1 x_2 = 0$$
$$g(x) = x^2 \quad \omega_0 x_1^2 + \omega_1 x_2^2 = \frac{\sqrt{\pi}}{2}$$
$$g(x) = x^3 \quad \omega_0 x_1^3 + \omega_1 x_2^3 = 0$$

Solving these 4 equations, we'll get

$$x_1 = \frac{1}{2}\sqrt{2}$$

$$x_2 = -\frac{1}{2}\sqrt{2}$$

$$\omega_1 = \frac{1}{2}\sqrt{\pi}$$

$$\omega_2 = \frac{1}{2}\sqrt{\pi}$$

# 2 Algorithm

# Algorithm 1 n-point Gauss Hermite Quadrature rulefunction MyHermiteQuad(f, n) $\triangleright$ Store the x values and weights in two lists $[herm\_zer, w] = h\_roots(n)$ $\triangleright$ Store the x values and weights in two listsherm = 0 $\triangleright$ initialize the summationfor i in range(1, n+1): $herm + f(herm\_zer[i-1]) * w[i-1]$ $\triangleright$ loop to sum all values for the integralreturn herm $\triangleright$ Returns the value of integral

# 3 Programming

```
#Ankur Kumar 2020PHY1113
2 #Preetpal Singh 2020PHY1140
5 from IntegrationModule import *
6 from scipy.integrate import quad
7 import numpy as np
8 import pandas as pd
9 from prettytable import PrettyTable
print("2020PHY1113")
13
14 ver_f = eval("lambda x:" + input("function to be integrated by Gauss Hermite , f(x))
16 x = PrettyTable()
17
x.field_names = ["n-point", "Inbuilt Function", "My Function"]
20 x.add_row(["2", quad(lambda x: np.exp(-(x**2))*ver_f(x), -np.inf, np.inf)[0],
      MyHermiteQuad(ver_f, 2)])
21 x.add_row(["4", quad(lambda x: np.exp(-(x**2))*ver_f(x), -np.inf, np.inf)[0],
      MyHermiteQuad(ver_f, 4)])
22
23 print(x)
24
25 def Int_1(x):
     return 1/(1+x**2)
26
27
28 def Int_2(x):
      return np.exp(x**2)/(1+x**2)
31 I1 = []
32 I2 = []
33 n = []
34 for i in range(1, 8):
      val_1 = MyHermiteQuad(Int_1, 2**i)
      I1.append(val_1)
36
37
38
39 for i in range(1, 8):
      val_2 = MyHermiteQuad(Int_2, 2**i)
      I2.append(val_2)
41
      n.append(2**i)
43
44 data = {
```

```
46 'n': n,
47 'I_1': I1,
    'I_2': I2
48
49
50 }
51
52 df = pd.DataFrame(data)
numpy_array = df.to_numpy()
54 np.savetxt("quad-herm-1113.out.txt", numpy_array, fmt = "%f")
57
58 #Comparsion With Simpson Method
func_1 = lambda x: np.exp(-(x**2))/(1+x**2)
func_2 = lambda x: 1/(1+x**2)
63 \text{ simp1} = []
64 \text{ simp2} = []
65 upperLimit = []
66 lowerLimit = []
68 for i in range(0,5):
69
       temp1 = My_Simp(func_1, -10**i, 10**i, 100000)
70
71
       simp1.append(temp1)
72
      temp2 = My_Simp(func_2, -10**i, 10**i, 100000)
73
      simp2.append(temp2)
74
75
       temp3 = 10**i
76
      upperLimit.append(temp3)
77
78
      temp4 = -10**i
79
80
      lowerLimit.append(temp4)
81
82
83 data1 = {
      'Lower Limit': lowerLimit,
84
    'Upper Limit': upperLimit,
'I_1(Simpson)': simp1,
85
86
87
    'I_2(Simpson)': simp2
88
89 }
91 df = pd.DataFrame(data1)
92 print(df)
```

### 4 Discussion

## Verification of n-point Gauss Hermite

We know that for n-point Gauss Hermite the method will give exact results upto 2n-1 order of polynomials.

For n=2 the integral is exact upto 3rd order polynomials.

For n = 4 the integral is exact upto 7th order polynomials.

```
function to be integrated by Gauss Hermite , f(x) = x**2
+-----+
| n-point | Inbuilt Function | My Function |
+-----+
| 2 | 0.8862269254527599 | 0.8862269254527577 |
| 4 | 0.8862269254527599 | 0.8862269254527573 |
+-----+
```

Figure 1: Polynomial of Order 2

For the given 2nd order polynomial it can be seen that both 2-point and 4-point quadrature gives exact results.

```
function to be integrated by Gauss Hermite , f(x) = x**6
+-----+
| n-point | Inbuilt Function | My Function |
+-----+
| 2 | 3.3233509704478426 | 0.22155673136318937 |
| 4 | 3.3233509704478426 | 3.323350970447833 |
+-----+
```

Figure 2: Polynomial of Order 6

For the given 6th order polynomial it can be seen that 2-point quadrature fails to give an exact result and 4-point is still accurate as predicted.

Figure 3: Polynomial of Order 8

For the given 8th order polynomial it can be seen that both 2-point and 4-point quadrature fail to give exact results.

# Evaluating $I_1$ and $I_2$

Figure 4: Value of Integrals with change in n

It can be seen that as value of n increases the value of integral approaches the true value, but the second integral does not reach the true value of  $\pi$  even with 128 point quadrature.

## Computation using two-point quadrature

### Integral I

$$f(x) = \frac{1}{1+x^2}$$

$$I_{1} = \sum_{i=1}^{N} w_{i} f(x_{i})$$

$$I_{1} = w_{1} f(x_{1}) + w_{2} f(x_{2})$$

$$I_{1} = \frac{\sqrt{\pi}}{2} f\left(\frac{1}{\sqrt{2}}\right) + \frac{\sqrt{\pi}}{2} f\left(\frac{-1}{\sqrt{2}}\right)$$

$$I_{1} = (0.886227)(0.666667) + (0.886227)(0.666667)$$

$$I_{1} = 1.181636$$

#### Integral II

$$f(x) = \frac{e^{x^2}}{1+x^2}$$

$$I_{1} = \sum_{i=1}^{N} w_{i} f(x_{i})$$

$$I_{1} = w_{1} f(x_{1}) + w_{2} f(x_{2})$$

$$I_{1} = \frac{\sqrt{\pi}}{2} f\left(\frac{1}{\sqrt{2}}\right) + \frac{\sqrt{\pi}}{2} f\left(\frac{-1}{\sqrt{2}}\right)$$

$$I_{1} = (0.886227)(1.099148) + (0.886227)(1.099148)$$

$$I_{1} = 1.948188$$

# Comparison with Simpson Method

	Lower Limit	Upper Limit	<pre>I_1(Simpson)</pre>	<pre>I_2(Simpson)</pre>
0	-1	1	1.237644	1.570796
1	-10	10	1.343293	2.942255
2	-100	100	1.343293	3.121593
3	-1000	1000	1.343293	3.139593
4	-10000	10000	1.343293	3.141393

Figure 5: Comparison with Simpson Method

We change the values of both upper limit and lower limit towards infinity.

It can be seen that as the value of upper limit and lower limit goes on increasing both the integrals approach their true value.

With this method the value of second integral can be approximated to  $\pi$ .