The Gaussian Quadrature

In Lecture 5, we explored the three fundamental methods for computing definite integrals numerically: by use of rectangles, the Trapezoid Rule, and Simpson's Rule. We also found that the third method, Simpson's Rule, is superior to the other two methods when it comes to obtaining accurate approximation of any integral. Therefore, if we know how to use Simpson's Rule, there's really no reason for us to even bother using the rectangle method or the Trapezoid Rule as they are obsolete.

However, there is a fourth method that wasn't explicitly mentioned: $The\ Gaussian\ Quadrature\ Rule$. Like with Simpson's Rule, we may be asking "Is this method better than even Simpson's Rule?". The short answer to this question is yes, and we will see later by looking at some examples.

The $Gaussian\ Quadrature\ Rule$ was named after Carl Friedrich Gauss, and it was meant to produce exact results for polynomials of degree $2n-1$ or less by a suitable choice of the nodes x_i and weights w_i for $i = 1, 2, 3, \ldots, n$(Wikipedia). Whereas the rectangle, Trapezoid, and Simpson's rule all require that the width(Δx) be the same, the Gaussian Quadrature Rule dictates that the opposite is more suitable: unequal widths will give better approximation.

So how does the $Gaussian\ Quadrature\ Rule$ work? Suppose we have a function that we want to integrate over the interval $[a, b]$. Let that function be a function of x and let the area under the curve of that function be denoted by A. Then,

$$(1)\ A = \int_a^b f(x)dx$$

As we can see, f is being integrated over the interval $[a, b]$. We need to shift this interval into the following

$$[a, b] \implies [-1, 1]$$

before the Gaussian Quadrature method can work. We will do this in the next section.

Shift(Change) of Interval

The interval of integration for Equation 1 must be changed from $[a, b]$ to $[-1, 1]$. Once we do this, the general form of the Gaussian Quadrature Rule will take the following

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}t + \frac{a+b}{2}\right)dt \text{ for all } t \in [-1, 1]$$

However, the right side is still an integral. Our goal is to transform it into an equivalent sum. We can do so by replacing the right side of this equation with something that transforms the whole thing into the following

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Where w_i is/are the weights, which are specific to the number of points n used, and x_i are the coefficients, which are also specific to the number of points used.

Finding Weights and Coefficients

The following rule, if I didn't already mention,

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

is exact for polynomials of degree $2n-1$, as I mentioned in the beginning. This rule has a special name, $Gauss - Legendre\ Quadrature\ Rule$. This rule will only be an accurate approximation to the integral above if $f(x)$ is well-approximated by a polynomial of degree $2n-1$ or less on $[-1,1]$(Wikipedia). Again, w_i are the weights, which are unique to the number of points that we choose to use. While this goal may seem difficult, it actually is not. This can be approached by either using Linear Algebra without Calculus, or using Calculus without Linear Algebra. We will do the latter.

The general rule for finding the weights w_i is given by

$$w_i = \frac{2}{(1-x_i^2)[P_n'(x_i)]^2}$$

where $P_n(x)$ is the $Legendre - Polynomial$. To make this rule useful and how we can find all w_i's and x_i's, we use Calculus.

Let I be the integral representing the area under the curve of some function $f(x)$. This means

$$I = \int_a^b f(x)dx = w_1 f(x_1) + w_2 f(x_2) + \ldots + w_n f(x_n) = \sum_{i=1}^{n} w_i f(x)$$

We then do the following:

$$\begin{aligned}
f(x) = 1 &\implies \int_{-1}^{1} 1dx = w_1 f(x_1) + w_2 f(x_2) = 2 \\
f(x) = x &\implies \int_{-1}^{1} xdx = w_1 f(x_1) + w_2 f(x_2) = 0 \\
f(x) = x^2 &\implies \int_{-1}^{1} x^2dx = w_1 f(x_1) + w_2 f(x_2) = \frac{2}{3} \\
f(x) = x^3 &\implies \int_{-1}^{1} x^3dx = w_1 f(x_1) + w_2 f(x_2) = 0
\end{aligned}$$

If we clean things up by rearranging, we get

$$\begin{aligned}
w_1 f(x_1) + w_2 f(x_2) &= 2 \\
w_1 f(x_1) + w_2 f(x_2) &= 0 \\
w_1 f(x_1) + w_2 f(x_2) &= \frac{2}{3} \\
w_1 f(x_1) + w_2 f(x_2) &= 0
\end{aligned}$$

We have four equations and four unknowns. The four unknowns are readily obtainable by performing typical row-operations with Linear Algebra. Upon performing the row-operations, we get that

$$w_0 = w_1 = 1 \text{ and } x_0 = -\frac{1}{\sqrt{3}} \text{ and } x_1 = \frac{1}{\sqrt{3}}$$

What we have actually obtained here is only applicable to two points of evaluation. Usually, we will need more than two points to get great results whenever we are applying the $Gaussian\ Quadrature\ Rule$. We can repeat what we did and generalize things for up to four points. Below are the suitable w_i's and x_i's for a given number of points n.

n = 2

$$w_1 = 1 \text{ and } x_1 = -1/\sqrt{3}$$
$$w_2 = 1 \text{ and } x_2 = 1/\sqrt{3}$$

n = 3

$$w_1 = 5/9 \text{ and } x_1 = -\sqrt{3/5}$$
$$w_2 = 8/9 \text{ and } x_2 = 0$$
$$w_3 = 5/9 \text{ and } x_3 = \sqrt{3/5}$$

n = 4

$$w_1 = (18 - \sqrt{30})/36 \text{ and } x_1 = -\sqrt{525 + 70\sqrt{30}}/35$$
$$w_2 = (18 + \sqrt{30})/36 \text{ and } x_2 = -\sqrt{525 - 70\sqrt{30}}/35$$
$$w_3 = (18 + \sqrt{30})/36 \text{ and } x_3 = \sqrt{525 - 70\sqrt{30}}/35$$
$$w_4 = (18 - \sqrt{30})/36 \text{ and } x_4 = \sqrt{525 + 70\sqrt{30}}/35$$

The list goes on. The bigger the value of n, the better the approximation becomes.

In [19]:

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from math import exp
from scipy.integrate import quad
%matplotlib inline

def p(x, n): # Legendre Polynomials up to p_8
    if n == 0:
        return 1
    elif n == 1:
        return x
    elif n == 2:
        return (1/2)*(3*x**2 - 1)
    elif n == 3:
        return (1/2)*(5*x**3 - 3*x)
    elif n == 4:
        return (1/8)*(35*x**4 - 30*x**2 + 3)
    elif n == 5:
        return (1/8)*(63*x**5 - 70*x**3 + 15*x)
    elif n == 6:
        return (1/16)*(231*x**6 - 315*x**4 + 105*x**2 - 5)
    elif n == 7:
        return (1/16)*(429*x**7 - 693*x**5 + 315*x**3 - 35*x)
    elif n == 8:
        return (1/128)*(6435*x**8 - 12012*x**6 + 6930*x**4 - 1260*x**2

def Gauss(f, a, b, n): # for  2 <= n <= 4
    if n == 2:
        wi = np.array([1, 1])
        xi = np.array([-1/3**(.5), 1/3**(.5)])
    elif n == 3:
        wi = np.array([5/9, 8/9, 5/9])
        xi = np.array([-(3/5)**.5, 0, (3/5)**.5])
    elif n == 4:
        c0 = (18 - np.sqrt(30))/36
        c1 = (18 + np.sqrt(30))/36
        c2 = c1
        c3 = c0
        x2 = np.sqrt(525 - 70*np.sqrt(30))/35
        x3 = np.sqrt(525 + 70*np.sqrt(30))/35
        x0 = -x3
        x1 = -x2
        wi = np.array([c0, c1, c2, c3])
        xi = np.array([x0, x1, x2, x3])
    return ((b - a)/2)*sum(wi*f((b - a)/2*xi + (a + b)/2))

def integral(function, lower, upper, n, method = 'Rectangle'):
    Sum = 0
    deltaX = (upper - lower)/n
    if method == 'Rectangle':
        x = np.linspace(lower, upper, n)
        for i in x:
            Sum = Sum + function(i)
        area = deltaX*Sum
        return area
```

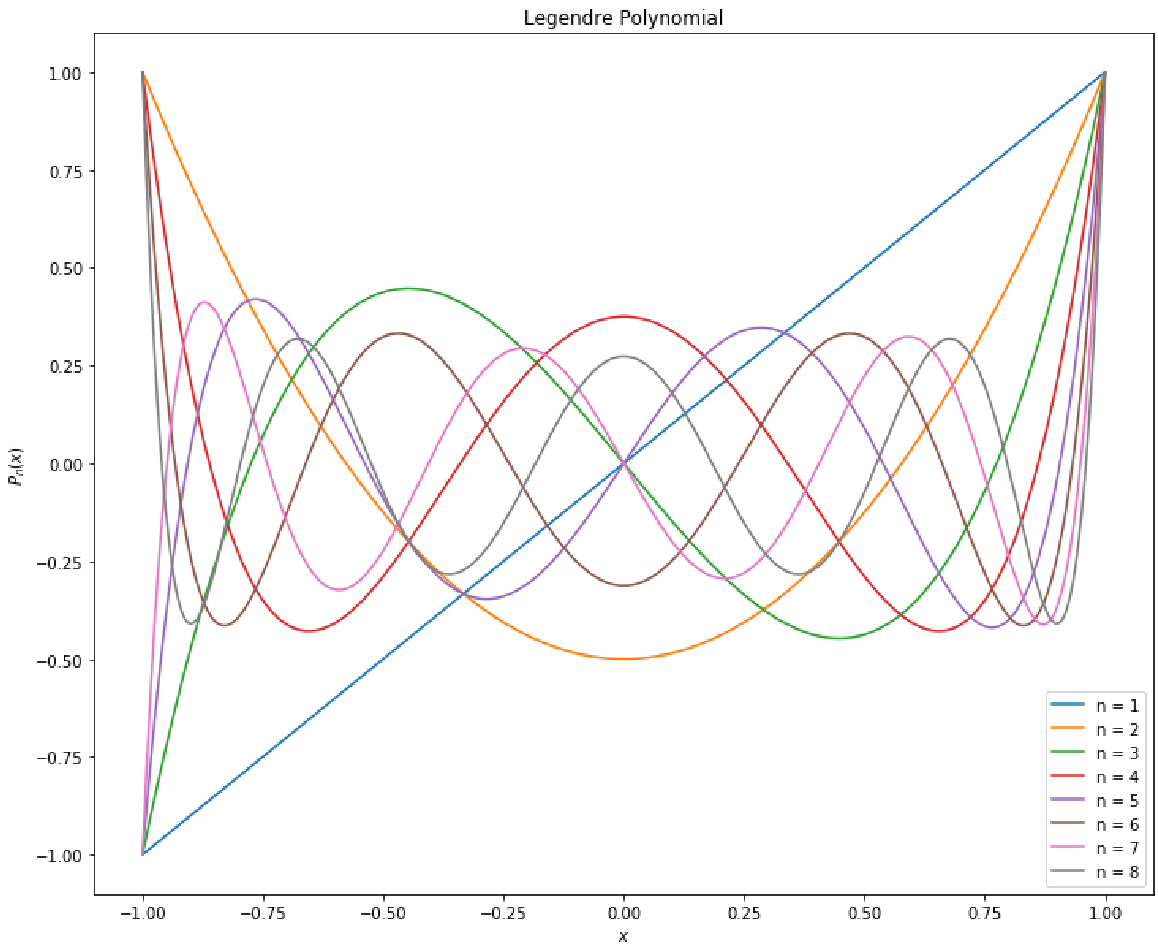
```
    elif method == 'Trapezoid':
        x1 = lower
        x2 = x1 + deltaX
        while x2 <= upper:
            Sum = Sum + (deltaX/2)*(function(x1) + function(x2))
            x1 = x2
            x2 = x1 + deltaX
        return Sum
    elif method == 'Simpson':
        x1 = lower
        x2 = x1 + deltaX
        x3 = x2 + deltaX
        while x3 <= upper:
            Sum = Sum + (deltaX/3)*(function(x1) + 4*function(x2) + fur
            x1 = x3
            x2 = x1 + deltaX
            x3 = x2 + deltaX
        return Sum
    else:
        print('Choose a method from any of the following: Rectangle, Tr
        return None

def root(f, initial):
    x0 = initial
    if f(x0) > 0:
        while f(x0) > 0:
            x0 = x0 - 0.00001
    elif f(x0) < 0:
        while f(x0) < 0:
            x0 = x0 - 0.00001
    return x0

def derivative(f, x):
    h = 0.000000000000001
    return (f(x + h) - f(x))/h

def wi(f, xi):
    den = (1 - xi**2)*(derivative(f, xi))**2
    return 2/den
wi = np.vectorize(wi)
root = np.vectorize(root)
```

Legendre Polynomial

Below is a graph of the Legendre Polynomial in the interval $-1 \leq x \leq 1$ for $1 \leq n \leq 8$.

In [4]:

```
x = np.linspace(-1, 1, 1000)
Labels = ['n = 0', 'n = 1', 'n = 2', 'n = 3', 'n = 4', 'n = 5', 'n = 6'
plt.figure(figsize = (12, 10))
for i in range(1, 9, 1):
    plt.plot(x, p(x, i), label = Labels[i])
plt.xlabel('$ x $')
plt.ylabel('$ P_n(x) $')
plt.title('Legendre Polynomial')
plt.legend()
plt.show()
```



Gaussian Quadrature, scipy, and Simpson's Rule(Comparison)

Let us test the three methods on the integral

$$\int_1^2 \left(2x + \frac{3}{x}\right)^2 dx$$

In [72]:

```
f = lambda x: (2*x + 3/x)**2
from scipy.integrate import quad
print('scipy.integrate.quad:', quad(f, 1, 2)[0])
print('Gaussian Quadrature with 4 points:', Gauss(f, 1, 2, 4))
print("Simpson's Rule:", integral(f, 1, 2, 1000, method = 'Simpson'))
```

```
scipy.integrate.quad: 25.833333333333332
Gaussian Quadrature with 4 points: 25.833289661396922
Simpson's Rule: 25.833333333333993
```

Speed Comparison

In [74]:

```
%timeit quad(f, 1, 2)[0]
%timeit Gauss(f, 1, 2, 4)
%timeit integral(f, 1, 2, 1000, method = 'Simpson')
```

```
9.61 µs ± 330 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
18.3 µs ± 611 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
653 µs ± 46.1 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

The Gaussian Quadrature method is a little less than half(1.9 times) as fast as the built-in function $quad$, but it is still much faster than $Simpson's\ Rule$ at almost 36 times the speed its speed, and considering that we didn't have to use as many points as we did using Simpson's Rule and still get an accurate answer, it goes to show just how good the Gaussian Quadrature method is. Let us try another example.

$$\int_{0.1}^{1.3} 5xe^{-2x}\,dx$$

In [78]:

```
f = lambda x: 5*x*np.exp(-2*x)
print('scipy.integrate.quad:', quad(f, 0.1, 1.3)[0])
print('Gaussian Quadrature with 4 points:', Gauss(f, 0.1, 1.3, 4))
print("Simpson's Rule:", integral(f, 0.1, 1.3, 1000, method = 'Simpson'
```

```
scipy.integrate.quad: 0.8938650276524702
Gaussian Quadrature with 4 points: 0.8938681930382849
Simpson's Rule: 0.8927046475426311
```

In [80]:

```
%timeit quad(f, .1, 1.3)[0]
%timeit Gauss(f, .1, 1.3, 4)
%timeit integral(f, 0.1, 1.3, 1000, method = 'Simpson')
```

```
23.9 µs ± 924 ns per loop (mean ± std. dev. of 7 runs, 10000 loops each)
17.7 µs ± 122 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
1.82 ms ± 43.9 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

General Form of Gaussian Quadrature

The code above only works for Gaussian integration of up to 4 points. However, to truly surpass the accuracy obtained by Simpson's Rule, we need to use more than 4 points with the Gaussian Quadrature Rule. In Lecture 5 - Integrals, we were given the code that calculates the Gaussian Quadrature method for any order n of the Legendre Polynomials. Recall from earlier that the area under any curve is given by

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

The description of the parameters is as follows

(i) x_i is the ith root of the required Legendre Polynomial which can be found by Newton's m

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

(ii) w_i is the corresponding ith weight of x_i given by the formula

$$w_i = \frac{2}{(1-x_i^2)[P_n'(x_i)]^2}$$

In [23]:

```
from numpy import ones,copy,cos,tan,pi,linspace

def gaussxw(N):

    # Initial approximation to roots of the Legendre polynomial
    a = linspace(3,4*N-1,N)/(4*N+2)
    x = cos(pi*a+1/(8*N*N*tan(a)))

    # Find roots using Newton's method
    epsilon = 1e-15
    delta = 1.0
    while delta>epsilon:
        p0 = ones(N,float)
        p1 = copy(x)
        for k in range(1,N):
            p0,p1 = p1,((2*k+1)*x*p1-k*p0)/(k+1)
        dp = (N+1)*(p0-x*p1)/(1-x*x)
        dx = p1/dp
        x -= dx
        delta = max(abs(dx))

    # Calculate the weights
    w = 2*(N+1)*(N+1)/(N*N*(1-x*x)*dp*dp)

    return x,w


def f(x):
    return x**5 - 2*x + 1

# finalizes the calculation of the area under the curve
def GaussArea(f, a, b, n):
    x, w = gaussxw(n)
    xp = 0.5*(b - a)*x + 0.5*(b + a)
    wp = 0.5*(b - a)*w
    return sum(wp*f(xp))
```

Let us perform some integration comparison between three methods on the integral

$$\int_0^2 (x^5 - 2x + 1)dx$$

.

In [52]:

```python
import pandas as pd
n = 30
a, b = 0, 2
f = lambda x: x**5 - 2*x + 1
index = [i for i in range(1, 31, 1)]
simpson = np.empty(30, dtype = float)
gauss = np.empty(30, dtype = float)
Scipy = np.empty(30, dtype = float)
for i in index:
    simpson[i - 1] = integral(f, a, b, n, method = 'Simpson')
    gauss[i - 1] = GaussArea(f, a, b, n)
    Scipy[i - 1] = quad(f, a, b)[0]


Index = [3, 10, 100, 2000, 3000, 30000]
for i in Index:
    print('For n =', i)
    print('
    print("Simpson's Rule:", integral(f, a, b, i, method = 'Simpson'))
    print("Gaussian QuadR:", GaussArea(f, a, b, i))
    print("Scipy.Int.Quad:", quad(f, a, b)[0])
    print('
    print('
    print('
```

```
For n = 3

Simpson's Rule: 0.6090534979423866
Gaussian QuadR: 8.666666666666684
Scipy.Int.Quad: 8.666666666666666



For n = 10

Simpson's Rule: 8.668799999999996
Gaussian QuadR: 8.666666666666746
Scipy.Int.Quad: 8.666666666666666



For n = 100

Simpson's Rule: 7.567385600768027
Gaussian QuadR: 8.666666666666647
Scipy.Int.Quad: 8.666666666666666



For n = 2000

Simpson's Rule: 8.666666666665758
Gaussian QuadR: 8.666666666666673
Scipy.Int.Quad: 8.666666666666666
```

```
For n = 3000

Simpson's Rule: 8.666666666665343
Gaussian QuadR: 8.666666666666679
Scipy.Int.Quad: 8.666666666666666


For n = 30000

Simpson's Rule: 8.666666666661781
Gaussian QuadR: 8.666666666666714
Scipy.Int.Quad: 8.666666666666666
```

We can see above that even for smaller values of n, like $n \leq 10$, the Gaussian Quadrature Rule outperforms Simpson's Rule in terms of accurary every single time if significant digits is taken into consideration. The purpose of the Gaussian Quadrature Rule is to be able to use as less points as possible so Python can run at maximum speed, while still getting very very accurate area approximation under the curve. As we have seen above, even with $n = 30,000$, Simpson's Rule cannot match the accurate area value given by the Gaussian Quadrature Rule with only $n = 3$.

Speed Test

Let us compare the speed of Simpson's Rule with $n = 30,000$ and Gaussian Quadrature Rule with $n = 3$.

In [53]:

```
%timeit GaussArea(f, a, b, 3)
%timeit integral(f, a, b, 30000, method = 'Simpson')
```

```
567 µs ± 11.1 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
20.2 ms ± 876 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

As we can see here, the Gaussian Quadrature is over 35 times faster than Simpson's Rule and is also much more accurate. Let us integrate another function as another example. Consider

$$\int_{0.5}^{1.5} e^x cos(x)dx$$

In [54]:

```
f = lambda x: np.exp(x)*np.cos(x)
Index = [3, 10, 100, 2000, 3000, 30000]
for i in Index:
    print('For n =', i)
    print('
    print("Simpson's Rule:", integral(f, a, b, i, method = 'Simpson'))
    print("Gaussian QuadR:", GaussArea(f, a, b, i))
    print("Scipy.Int.Quad:", quad(f, a, b)[0])
    print('
    print('
    print('
```

```
For n = 3

Simpson's Rule: 1.7811579356552514
Gaussian QuadR: 1.320753212370422
Scipy.Int.Quad: 1.3219586883944454



For n = 10

Simpson's Rule: 1.3219098617857168
Gaussian QuadR: 1.3219586883944339
Scipy.Int.Quad: 1.3219586883944454



For n = 100

Simpson's Rule: 1.437263498310077
Gaussian QuadR: 1.3219586883944472
Scipy.Int.Quad: 1.3219586883944454



For n = 2000

Simpson's Rule: 1.3219586883947458
Gaussian QuadR: 1.3219586883944463
Scipy.Int.Quad: 1.3219586883944454



For n = 3000

Simpson's Rule: 1.3219586883946683
Gaussian QuadR: 1.3219586883944494
Scipy.Int.Quad: 1.3219586883944454



For n = 30000

Simpson's Rule: 1.3219586883951966
```

```
Gaussian QuadR: 1.3219586883944505
Scipy.Int.Quad: 1.3219586883944454
```

This is almost the same exact thing that happened with the previous example. Gaussian Quadrature Rule evaluated at only 10 points beats Simpson's Rule with $30,000$ points. This concludes my project.