

Lecture 12 - A

§5.4 Gaussian Quadrature

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We will answer these questions:

- What is **degree of precision**?
- In what way are **Newton-Cotes methods** restrictive?
- What is the main idea behind **Gaussian quadrature**?
- How does its **performance** compare?



Degree of Precision



Degree of Precision

Definition: Degree of Precision

Suppose an integration method has zero error when applied to a polynomial $p_r(x)$ (assume r is the highest degree). Then we say the method has **degree of precision** equal to r .

Note

Do not confuse **order of accuracy** p ($E = \mathcal{O}(h^p)$) with degree of precision r . They are both integers and they are both related to performance of a method.

Question

What is the degree of precision for the Newton-Cotes integration methods?



Degree of Precision

Trapezoid

Example

- Find the exact integral of $y = f(x) = 2x + 1$ on $[1, 3]$.
- Approximate $\int_1^3 f(x) dx$ using the basic trapezoid.
- The exact integral is

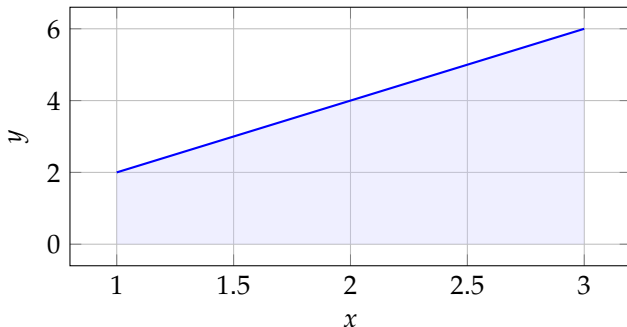
$$\int_1^3 2x + 1 dx = x^2 + x \Big|_1^3 = 8 + 2 = 10$$

- The trapezoid approximation is

$$\int_1^3 2x + 1 dx \approx \frac{f(3) + f(1)}{2} (3 - 1) = \frac{7 + 3}{2} (2) = 10$$

Note

Degree of precision for Trapezoid method is $r = 1$.



- The integral $\int_1^3 (2x + 1) dx$ is the area of a trapezoid
- This is always true when integrating a linear function

Key Idea

Trapezoid Method has **no error** for linear functions.

Degree of Precision

Newton-Cotes

- Recall that Newton-Cotes approximates $f(x) \approx p_n(x)$ and then integrates

$$I = \int_a^b f(x) dx \approx \int_a^b p_n(x) dx$$

- If $f(x) = p_n(x)$, then there cannot be any error

$$E = \int_a^b f(x) dx - \int_a^b p_n(x) dx = \int_a^b f(x) - p_n(x) dx = 0$$

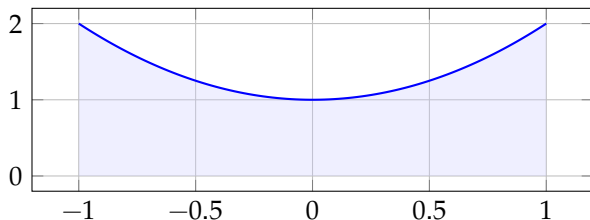
- Therefore

Note

A Newton-Cotes method of degree n has a degree of precision of at least n , and sometimes higher.



Simpson's Rule



- Simpson's rule says

$$\int_{-1}^1 f(x) dx \approx \frac{1}{3}(f(-1) + 4f(0) + f(1))$$

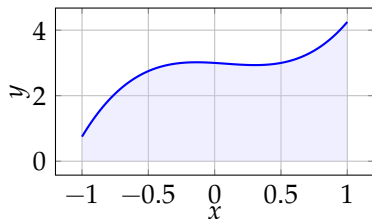
- If we apply it so $f(x) = x^2 + 1$ then we get

$$\int_{-1}^1 f(x) dx \approx \frac{1}{3}(2 + 4 + 2) = \frac{8}{3}$$

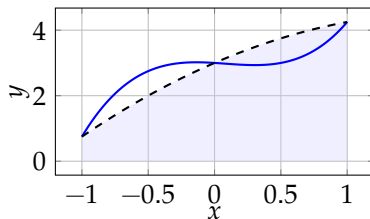
- This is **exact!**



Degree of Precision for Simpson's



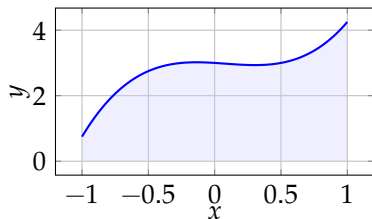
$$\int_{-1}^1 x(x-0.5)(x+0.5) + 3 \, dx$$



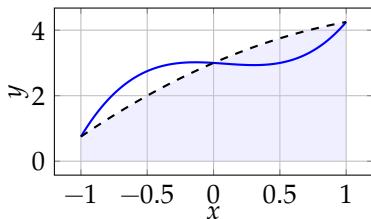
$$\int_{-1}^1 p_2(x) \, dx$$

- We know degree of precision is at least 2

Degree of Precision for Simpson's



$$\int_{-1}^1 x(x-0.5)(x+0.5) + 3 dx$$



$$\int_{-1}^1 p_2(x) dx$$

- We know degree of precision is at least 2
- Actually, the degree of precision is 3 - Verify this for Homework!

$$\int_{-1}^1 x(x-0.5)(x+0.5) + 3 dx = \int_{-1}^1 p_2(x) dx$$

Derivatives in the Error Formulas

- Trapezoid $-\frac{(b-a)h^2}{12}f''(\xi)$

degree of precision = 1

- Simpson's 1/3 $-\frac{(b-a)h^4}{90}f^{(4)}(\xi)$

degree of precision = 3

- Simpson's 3/8 $-\frac{(b-a)h^4}{80}f^{(4)}(\xi)$

degree of precision = 3

- Boole's $-\frac{2(b-a)h^6}{945}f^{(6)}(\xi)$

degree of precision = 5



Gaussian Quadrature



Definition: Quadrature

- **Numerical Quadratures** are integration rules that can be expressed as the weighted sum

$$\int_a^b f(x) dx \approx \sum_{i=0}^n w_i f(x_i)$$

- The w_i are called **weights**, the x_i are called **nodes**
- Newton-Cotes rules are quadratures with **equispaced nodes**

$$x_i = a + ih, \quad h = (b - a)/n$$

- Example: Simpson's Rule

$$\int_0^1 f(x) dx \approx \frac{1}{6}f(x_0) + \frac{2}{3}f(x_1) + \frac{1}{6}f(x_2)$$



Newton-Cotes

- Trapezoid

$$\frac{(b-a)}{2} [f(a) + f(b)]$$

- Simpson's 1/3

$$\frac{(b-a)}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

- Simpson's 3/8

$$\frac{(b-a)}{8} [f(a) + 3f(a+h) + 3f(b-h) + f(b)]$$

- Boole's

$$\frac{(b-a)}{90} \left[7f(a) + 32f(a+h) + 12f\left(\frac{a+b}{2}\right) + 32f(b-h) + 7f(b) \right]$$

Key Idea

Newton-Cotes are a subclass of quadratures with **equispaced** nodes.

Degrees of Freedom

General Quadrature

Definition: Degrees of Freedom

The number of free parameters in a numerical method is called the **degrees of freedom**.

Question

What is the degrees of freedom for a general quadrature with $n + 1$ nodes?

$$\sum_{i=0}^n w_i f(x_i) = \underbrace{w_0 f(x_0) + \cdots + w_n f(x_n)}_{n+1 \text{ terms}}$$

free *free*

- $n + 1$ weights
- $n + 1$ node locations
- Total: $2n + 2$



Degrees of Freedom

Newton-Cotes

Question

How many free variables are there in a Newton-Cotes quadrature with $n + 1$ nodes?

$$\sum_{i=0}^n w_i f(x_i) = \underbrace{\underbrace{w_0}_{\text{free}} \underbrace{f(x_0)}_{\text{fixed}} + \cdots + w_n f(x_n)}_{n+1 \text{ terms}}$$

- Node locations are *not* free
- They must be located at $x_i = a + \frac{b-a}{n}i$
- Newton-Cotes has only $n + 1$ free variables



Newton-Cotes vs. General Quadratures

- Newton-Cotes: $n + 1$ degrees of freedom
- General quadratures: $2n + 2$ degrees of freedom

Question

If we free up the location of the nodes, what can we with the extra degrees of freedom?

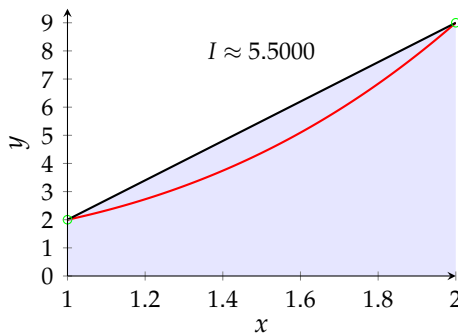
- We can add extra constraints.
- We can choose to optimize some quantity
- We can optimize a quadrature for **degree of precision!**



Cubic Function

Consider integrating the cubic function over the interval $[1, 2]$

$$f(x) = x^3 + 1$$



- The exact answer is 4.75
- Trapezoidal rule will yield 5.5 (overshoot)

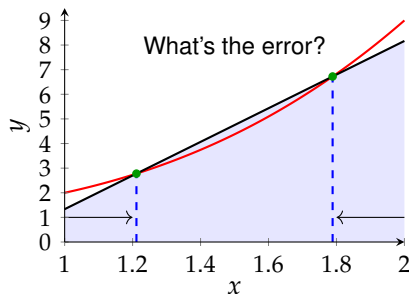
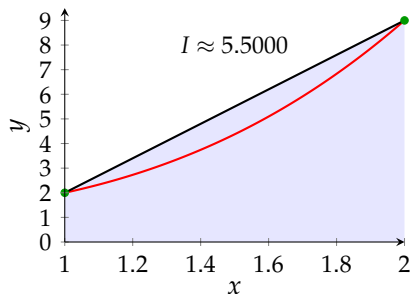


Cubic Function

Moving the Nodes

Consider

$$\int_1^2 x^3 + 1 \, dx = 4.75$$



Question

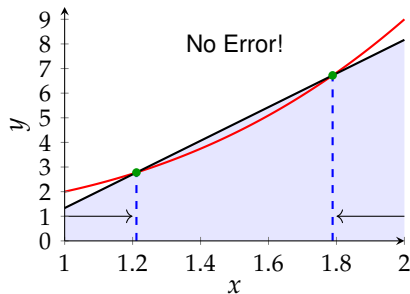
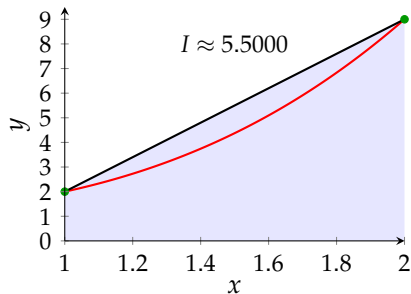
Can we move the nodes x_0 and x_1 inward so that the error is zero?

Cubic Function

Moving the Nodes

Consider

$$\int_1^2 x^3 + 1 dx = 4.75$$



Key Idea

Yes! We can achieve zero error with a trapezoid!

Method: Gaussian Quadrature

- **Given:** Integral $\int_a^b f(x) dx$, number of points $n + 1$
 - **Output:** Integral approximation
 - **Idea:** The quadrature weights w_i and nodes x_i are chosen to optimize the degree of precision.
-
- Gaussian Quadrature chooses w_i and x_i so that there is no error for polynomials

$$p_1(x), p_2(x), \dots, p_k(x)$$

where k is the highest possible degree



Two-point Gaussian Quadrature



Domain of Integration

- A general integral $\int_a^b f(x) dx$ can be over any interval.
- For simplicity, let's stick to the easy integral $[-1, 1]$.

Odd functions

If $f(x)$ is **odd** ($f(-x) = -f(x)$) then

$$\int_{-1}^1 f(x) dx = 0$$

Even functions

If $f(x)$ is **even** ($f(-x) = f(x)$) then

$$\int_{-1}^1 f(x) dx = 2 \int_0^1 f(x) dx$$



Gaussian Quadrature with $n = 1$

- Consider the case of $n = 1$ (2-points)
- Consider $[a, b] = [-1, 1]$ for simplicity

Goal

Let $p_k(x)$ be an arbitrary polynomial of degree k .
Choose w_0, w_1, x_0, x_1 so that

$$\int_{-1}^1 p_k(x) dx \approx w_0 p_k(x_0) + w_1 p_k(x_1)$$

has zero error for k as high as possible.



Gaussian Quadrature with $n = 1$

Let's try $p_1(x)$

- In general, $p_1(x) = ax + b$
- The exact integral is

$$\int_{-1}^1 p_1(x) dx = (0)a + (2)b \quad (*)$$

- The quadrature is

$$\begin{aligned} \int_{-1}^1 p_1(x) dx &= w_0 p_1(x_0) + w_1 p_1(x_1) \\ &= w_0(ax_0 + b) + w_1(ax_1 + b) \\ &= (w_0x_0 + w_1x_1)a + (w_0 + w_1)b \end{aligned} \quad (**)$$

- Since we need $(*) = (**)$, we have **2 conditions** and **4 unknowns**
- Infinite solutions



Gaussian Quadrature with $n = 1$

Let's try $p_2(x)$

- In general, $p_2(x) = ax^2 + bx + c$
- The exact integral is

$$\int_{-1}^1 p_2(x) dx = \frac{2}{3}a + 0b + 2c \quad (*)$$

- The quadrature is

$$\begin{aligned} \int_{-1}^1 p_2(x) dx &= w_0 p_2(x_0) + w_1 p_2(x_1) \\ &= w_0(ax_0^2 + bx_0 + c) + w_1(ax_1^2 + bx_1 + c) \\ &= (w_0x_0^2 + w_1x_1^2)a + (w_0x_0 + w_1x_1)b + (w_0 + w_1)c \quad (**) \end{aligned}$$

- we have **3 conditions** and **4 unknowns** $\implies$ infinite solutions



Degree of Precision for $n = 1$

Goal

Find the degree of precision for a simple quadrature of the form

$$\int_{-1}^1 f(x) dx \approx w_0 f(x_0) + w_1 f(x_1)$$

where the variables w_0 , w_1 , x_0 , and x_1 are all free.

- ✓ Degree ≥ 1
- ✓ Degree ≥ 2
- **Can we hit 3?**



Derivation

Part 1

Goal

Find w_0, w_1, x_0, x_1 so that the approximation

$$\int_{-1}^1 f(x) dx \approx w_0 f(x_0) + w_1 f(x_1)$$

is exact for any cubic function $f(x) = c_0 + c_1x + c_2x^2 + c_3x^3$.

- Exact integral

$$\int_{-1}^1 f(x) dx = \int_{-1}^1 (c_0 + c_1x + c_2x^2 + c_3x^3) dx$$

- The quadrature

$$w_0 f(x_0) + w_1 f(x_1) = w_0 (c_0 + c_1x_0 + c_2x_0^2 + c_3x_0^3) + w_1 (c_0 + c_1x_1 + c_2x_1^2 + c_3x_1^3)$$



Derivation

Part 2

- The exact integral is

$$\begin{aligned}\int_{-1}^1 f(x) \, dx &= \int_{-1}^1 (c_0 + c_1x + c_2x^2 + c_3x^3) \, dx \\ &= 2c_0 + 0c_1 + \frac{2}{3}c_2 + 0c_3\end{aligned}$$

- The quadrature is

$$\begin{aligned}w_0f(x_0) + w_1f(x_1) &= w_0(c_0 + c_1x_0 + c_2x_0^2 + c_3x_0^3) + w_1(c_0 + c_1x_1 + c_2x_1^2 + c_3x_1^3) \\ &= c_0(w_0 + w_1) + c_1(w_0x_0 + w_1x_1) + \cdots \\ &\quad c_2(w_0x_0^2 + w_1x_1^2) + c_3(w_0x_0^3 + w_1x_1^3)\end{aligned}$$

- We set the quadrature equal to the exact integral
- We set the factors of c_0 , c_1 , c_2 , and c_3 equal to get 4 equations



Derivation

Part 3

- Our equations are:

$$\begin{aligned}w_0 + w_1 &= 2 & w_0x_0 + w_1x_1 &= 0 \\w_0x_0^2 + w_1x_1^2 &= \frac{2}{3} & w_0x_0^3 + w_1x_1^3 &= 0\end{aligned}$$

- **4 equations** and **4 unknowns** $\implies$ there is a unique solution

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

Gaussian Quadrature with $n = 1$

$$\int_{-1}^1 f(x) \, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

Example 1

Example

Approximate $\int_{-1}^1 x^2 e^{-x} dx$ using Gaussian quadrature with $n = 1$.

- Using the weights $w_0 = w_1 = 1$ and points $x_0 = -\frac{\sqrt{3}}{3}$, $x_1 = \frac{\sqrt{3}}{3}$

$$\begin{aligned}\int_{-1}^1 f(x) dx &\approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) \\&= \left(-\frac{\sqrt{3}}{3}\right)^2 e^{\frac{\sqrt{3}}{3}} + \left(\frac{\sqrt{3}}{3}\right)^2 e^{-\left(\frac{\sqrt{3}}{3}\right)} \\&= \frac{1}{3} \left(e^{\frac{\sqrt{3}}{3}} + e^{-\left(\frac{\sqrt{3}}{3}\right)} \right) \approx 0.7809\end{aligned}$$



Change of Variables



Over general interval?

Warning!

The quadrature

$$\int_{-1}^1 f(x) dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

is only valid when integrating from -1 to 1 .

- That means we cannot directly use Gaussian quadrature to approximate integrals over general intervals

$$\int_a^b f(x) dx$$

- We can apply a **change of variables**. Let $x = \frac{b-a}{2}t + \frac{b+a}{2}$



Change of Variables in Integration

General Form

General Change of Variables

Let $x = g(t)$ be an invertible function. Then

$$\int_a^b f(x) dx = \int_{g^{-1}(a)}^{g^{-1}(b)} f(g(t))g'(t) dt$$

- If we let

$$x = g(t) = \frac{b-a}{2}t + \frac{b+a}{2}$$

- The inverse is $t = g^{-1}(x) = \frac{2x-(b+a)}{b-a}$ so

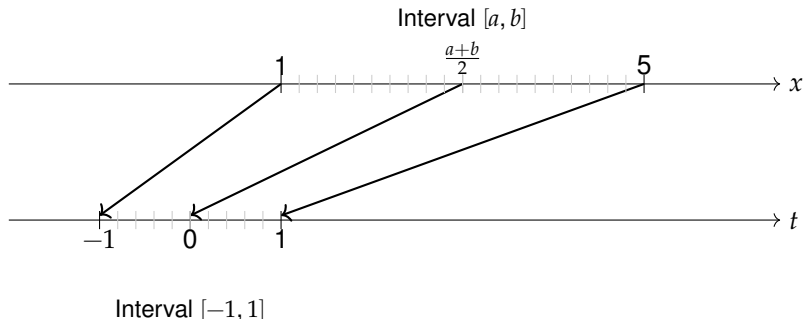
- $g^{-1}(b) = 1$
- $g^{-1}(a) = -1$

- The derivative is

$$g'(t) = \frac{b-a}{2}$$



Remapping the Interval



Change of Variables

The change of variables

$$t = g^{-1}(x) = \frac{2}{b-a}x - \frac{b+a}{b-a}$$

remaps an interval $x \in [a, b]$ to the interval $t \in [-1, 1]$.

Change of Variables in Integration

Applying to Gaussian Quadrature

Change of Variables Formula

Any integral over $[a, b]$ can be changed to an integral over $[-1, 1]$

$$\int_a^b f(x) dx = \int_{-1}^1 f \left(\underbrace{\frac{(b-a)t}{2} + \frac{b+a}{2}}_{u(t)} \right) \frac{b-a}{2} dt$$

Let us define this function $u(t)$.

2-point Gaussian Quadrature for $\int_a^b f(x) dx$

$$\int_a^b f(x) dx \approx \frac{b-a}{2} \left[u \left(-\frac{\sqrt{3}}{3} \right) + u \left(\frac{\sqrt{3}}{3} \right) \right], \text{ where}$$

$$u(t) = f \left(\frac{(b-a)t}{2} + \frac{b+a}{2} \right)$$

Example with Change of Interval

Example

Approximate $\int_1^2 (x^3 + 1) dx$ using Gaussian quadrature with $n = 1$.

- Apply the change of variables

$$\int_1^2 f(x) dx = \int_{-1}^1 f\left(\frac{(2-1)t + (2+1)}{2}\right) \frac{2-1}{2} dt$$

- Therefore, we are looking for the integral of

$$\frac{1}{2} \int_{-1}^1 f\left(\frac{t+3}{2}\right) dt = \frac{1}{2} \int_{-1}^1 \left(\frac{t+3}{2}\right)^3 + 1 dt$$

- Using Gaussian quadrature, our numerical integration becomes:

$$\frac{1}{2} \left[\left(\frac{\sqrt{3}/3 + 3}{2}\right)^3 + 1 + \left(\frac{-\sqrt{3}/3 + 3}{2}\right)^3 + 1 \right] = 4.75 \quad (\text{exact!})$$

- Standard Trapezoid Rule

$$\int_{-1}^1 f(x) dx \approx \frac{h}{2}f(-1) + \frac{h}{2}f(1)$$

- Gaussian Quadrature

$$\int_{-1}^1 f(x) dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

- Trapezoid is exact for **linear functions**, but Gauss is exact for **cubics**!



- General Gaussian Quadrature for $n + 1$ points
- Composite Gaussian Quadrature
- Derivation of Nodes and Weights

