## CS/SE 4X03 Tutorial Week 6 - Numerical Integration

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#### Exercise 1 - 5.1.1

#### **Recall: Composite Trapezoid Rule**

$$\int_{a}^{b} f(x)dx \approx T(f; P) = \frac{1}{2} \sum_{i=0}^{n-1} (x_{i+1} - x_i) [f(x_i) + f(x_{i+1})]$$

With uniform spacing,  $x_i = a + ih$  and  $h = \frac{b-a}{n}$  for i = 1, 2, ..., n-1:

$$\int_{a}^{b} f(x)dx \approx T(f; P) = \frac{h}{2} [f(x_0) + f(x_n)] + h \sum_{i=1}^{n-1} f(x_i)$$

## **Theorem 1 - Precision of Trapezoid Rule**

If f'' exists and is continuous on the interval [a,b] and if the composite trapezoid rule T with uniform spacing h is used to estimate the integral  $I = \int_a^b f(x) dx$ , then for some  $\zeta$  in (a,b),

$$I - T = -\frac{b - a}{12}h^2 f''(\zeta) = O(h^2)$$

Question: Compute an approximate value of:

$$\int_0^1 \frac{1}{x^2 + 1} \, \mathrm{d}x$$

by using the composite trapezoid rule with three points. Then compare with the actual value of the integral. Next, determine the error formula and numerically verify an upper bound on it.

Answer:

Given:

a=0: Lower bound of integral

b=1: Upper bound of integral

n = 3 - 1 = 2: Number of subintervals

 $h = \frac{b-a}{n} = 0.5$ : Spacing of subintervals

 $x_1 = 0.5$ : Our list of  $x_i$ , here just the midpoint of a and b

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

$$f^{(2)}(x) = \frac{6x^2 - 2}{(x^2 + 1)^3}$$
: 2<sup>nd</sup> derivative

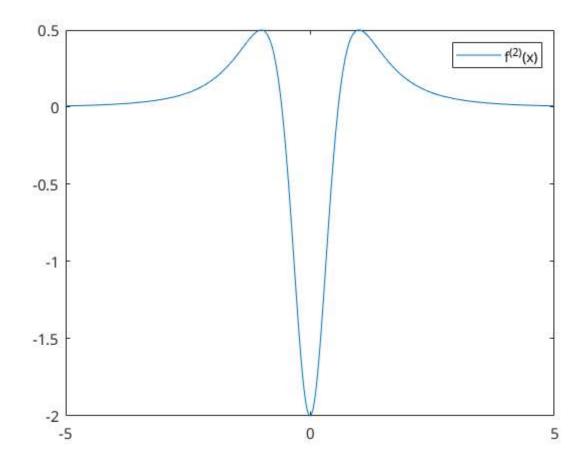
$$M = \max_{x \in [a,b]} |f^{(2)}(x)| = 2$$

```
clear all;
syms x;

f = 1/(1+x^2);
fp = simplify(diff(f,2))
```

fp = 
$$\frac{2 (3 x^2 - 1)}{(x^2 + 1)^3}$$

```
fplot(fp)
legend('f^{(2)}(x)')
```



$$f(a) = \frac{1}{1+0^2} = 1$$

$$f(x_i) = \frac{1}{1 + 0.5^2} = 0.8$$

$$f(b) = \frac{1}{1+1^2} = 0.5$$

Now using the composite trapezoid rule:

$$\int_{a}^{b} \approx h(0.5f(a) + 0.5f(b) + f(x_{1}))$$
$$= 0.5(0.5(1) + 0.5(0.5) + 0.5(0.8)) = 0.775000$$

We can compare this to analytical value:  $\arctan(1) = \frac{\pi}{4} \approx 0.785398$ 

$$error \approx 0.785398 - 0.775000 = 1.0398 \times 10^{-2}$$

Now using <u>Theorem 1</u>:

$$UBE = \frac{1}{12}(0.5)^2 \times 2 = 4.1667 \times 10^{-2}$$

**Note:** Just because Theorem 1 tells us a **bound** for the error, does not mean our error will be that large necessarily.

## **Exercise 2 - 5.1.6**

Question: Obtain an upper bound on the absolute error when we compute:

$$\int_0^6 \sin^2(x) dx$$

by means of the composite trapezoid rule using 101 equally spaced points.

**Answer:** 

Given:

a = 0: Lower bound of integral

b = 6: Upper bound of integral

n = 101 - 1 = 100: Subintervals

 $h = \frac{b-a}{n} = 0.06$ : Interval spacing

 $f(x) = \sin^2(x)$ : The function

 $f^{(2)}(x) = 2\cos(2x) : 2^{nd}$  derivative

$$M = \max_{x \in [a,b]} |f^{(2)}(x)| = 2 \max_{x \in [0,6]} |\cos(2x)| = 2$$

With our given information, we have enough to plug into <u>Theorem 1</u> and obtain a bound on our error:

$$UBE = \frac{6}{12}(0.06)^2 \times 2 = 3.6 \times 10^{-3}$$

## **Exercise 3 - 5.1.7**

**Question:** If the composite trapezoid rule is used to compute  $\int_{-1}^{2} \sin(x) dx$  with h = 0.01, give a realistic bound on the error.

Answer:

Given:

a = -1: Lower bound of integral

b = 2: Upper bound of integral

h = 0.01: Interval spacing

 $f(x) = \sin(x)$ : The function

 $f^{(2)}(x) = -\sin(x) : 2^{nd} \text{ derivative,}$ 

 $M = \max_{x \in [a,b]} |f^{(2)}(x)| = \max_{x \in [-1,2]} |-\sin(x)| = 1$ 

$$UBE = \frac{b-a}{12}h^2M$$

$$UBE = \frac{2 - (-1)}{12} \cdot 0.01^2 \times 1$$

$$UBE = 2.5 \times 10^{-5}$$

## **Exercise 4 - 5.1.8**

**Question:** How large must n be if the composite trapezoid rule is being used to estimate  $\int_0^{\pi} \sin(x) dx$  with  $error \le 10^{-12}$ ?

Answer: This time we are solving the inverse problem to the previous two exercises.

a=0: Lower bound of integral

 $b = \pi$ : Upper bound of integral

 $f(x) = \sin(x)$ : The function

$$f^{(2)}(x) = -\sin(x) : 2^{nd} \text{ derivative}$$

$$M = \max_{x \in [a,b]} |f^{(2)}(x)| = \max_{x \in [0,\pi]} |-\sin(x)| = 1$$

 $UBE \leq 10^{-12}$ 

Now we will consider that  $h = \frac{(b-a)}{n}$  to obtain:

$$UBE = \frac{b-a}{12}h^2M$$

$$UBE = \frac{(b-a)^3}{12n^2}M$$

Finally, we substitute and solve for *n* 

$$10^{-12} \ge \frac{(\pi - (0))^3}{12n^2} (1) = \frac{\pi^3}{12n^2}$$

$$n \ge 1607438$$

## Exercise 5 - 5.2.19

**Question:** Show that there exist coefficients  $w_0, w_1, ..., w_n$  depending on  $x_0, x_1, ..., x_n$  and on [a, b] such that:

$$\int_{a}^{b} p(x) \mathrm{d}x = \sum_{i=0}^{n} w_{i} p(x_{i})$$

for all polynomials p of degree  $\leq n$ .

Hint: Use the Lagrange form of the interpolating polynomial

**Answer:** We define  $L_i(x)$ , i = 0, 1, ..., n

$$L_i(x) = \prod_{j=0, j\neq i}^{n} \left(\frac{x - x_j}{x_i - x_j}\right), i = 0, 1, ..., n.$$

We can represent a polynomial using it's Lagrange interpolation:

$$p(x) = \sum_{i=0}^{n} f(x_i)L_i(x) = \sum_{i=0}^{n} p(x_i)L_i(x)$$

Integrating,

$$\int_{a}^{b} p(x)dx = \int_{a}^{b} \sum_{i=0}^{n} \left( p(x_i) L_i(x) dx \right)$$

But  $p(x_i)$  is independent of x:

$$= \sum_{i=0}^{n} \left( p(x_i) \int_{a}^{b} L_i(x) dx \right)$$

Thus we see:

$$\int_{a}^{b} p(x)dx = \sum_{i=0}^{n} p(x_i)w_i = \sum_{i=0}^{n} p(x_i) \int_{a}^{b} L_i(x)dx$$

and so:

$$w_i = \int_a^b L_i(x) dx$$

## **Exercise 6 - 5.2.1**

Recall: Basic Simpson's Rule

$$\int_{a}^{b} f(x)dx \approx S(f;P) = \frac{(b-a)}{6} \left[ f(a) + f(b) + 4f\left(\frac{a+b}{2}\right) \right]$$

And for the error we have:

$$error = -\frac{1}{90} \left( \frac{b-a}{2} \right)^5 f^{(4)}(\xi), \ \xi \in (a,b)$$

**Question:** Compute  $\int_0^1 \frac{1}{x^2 + 1} dx$  by the basic Simpson's Rule, using the three partition points x = 0, 0.5, 1. Compare with the true solution.

Answer: This is basically the first exercise, but now we want to do it using the Basic Simpson's Rule

a = 0: Lower bound of integral

b = 1: Upper bound of integral

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

$$f^{(4)}(x) = \frac{120x^4 - 240x^2 + 24}{(x^2 + 1)^5}$$
:  $2^{nd}$  derivative

$$M = \max_{x \in [a,b]} |f^{(4)}(x)| = 24$$

$$f(a) = \frac{1}{1+0^2} = 1$$

$$f\left(\frac{a+b}{2}\right) = \frac{1}{1+0.5^2} = 0.8$$

$$f(b) = \frac{1}{1+1^2} = 0.5$$

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{6} \left[ f(a) + f(b) + 4f\left(\frac{a+b}{2}\right) \right]$$
$$= \frac{1}{6} (1 + 0.8 \times 4 + 0.5) \approx 0.783333$$

We can compare this to analytical value:  $\arctan(1) = \frac{\pi}{4} \approx 0.785398$ 

$$error \approx 0.785398 - 0.783333 = 2.065 \times 10^{-3}$$

Note: This is better than the trapezoid rule

Now using the bound for error:

$$UBE = \frac{1}{2880}(b-a)^5 \max_{x \in [a,b]} |f^{(\cdot,\cdot)}(x)|$$

$$UBE = \frac{1}{2880}(1-0)^5 \times 24 \approx 8.333 \times 10^{-3}$$

This is indeed larger than an our error.

**Bonus:** In Questions 5.1.1 and 5.2.1, the *UBE*'s are all about 4 times of the corresponding actual error. Is this a coincidence? Or, is this caused by some properties of  $f(x) = 1/(1 + x^2)$ ? Think about it if you are willing to.

#### **Exercise 7 - 5.2.2**

**Question:** Consider the integral  $\int_0^{2\pi} \sin^2(x) dx$ . Suppose that we wish to integrate numerically, with an error of magnitude less than  $10^{-3}$ . What width h is needed if we wish to use the following rules?

1. Composite Trapezoid Rule

- 2. Composite Simpson's Rule
- 3. Composite Simpson's  $\frac{3}{8}$  Rule

Answer: This question is mostly just checking the error, and spacing required, for various rules

#### **Composite Trapezoid Rule:**

$$UBE = \frac{b - a}{12}h^2M = \frac{2\pi}{12}h^2 \times 2$$

Now we just solve for h when  $UBE \le 1 \times 10^{-3}$ 

$$UBE = \frac{\pi}{3}h^2 \le 0.003$$

$$\Rightarrow h \ge \sqrt{\frac{0.003}{\pi}} \approx 0.0309$$

#### Composite Simpson's Rule:

First we need the maximum of the fourth derivative:

$$f^{(4)}(x) = -8\cos(2x)$$

$$\Rightarrow \max_{x \in [a,b]} |f^{(4)}(x)| = 8$$

Now solve for h

$$UBE = \frac{1}{180}(b-a)h^4 \max_{x \in [a,b]} |f^{(4)}(x)| = \frac{4\pi}{45}h^4$$
$$\Rightarrow h \ge \sqrt[4]{\frac{0.045}{4\pi}} \approx 0.2446$$

# Composite Simpson's $\frac{3}{8}$ Rule

$$UBE = \frac{1}{80}(b-a)h^4 \max_{x \in [a,b]} |f^{(4)}(x)| = \frac{\pi}{5}h^4$$

Once again, we solve for *h*:

$$\frac{\pi}{5}h^4 \le 0.001$$

$$\Rightarrow h \ge \sqrt[4]{\frac{0.005}{4\pi}} \approx 0.1412$$

## Exercise 8 - 5.2.4

**Question:** Find an approximate value of  $\int_1^2 x^{-1} dx$  using composite Simpson's Rule with h = 0.25. Give a bound on the error.

#### **Answer:**

a = 1: Lower bound of integral

b = 2: Upper bound of integral

h = 0.25: Subinterval spacing

$$f(x) = \frac{1}{x}$$
: The function

$$f^{(4)}(x) = \frac{24}{x^5}$$
:  $4^{th}$  derivative

$$M = \max_{x \in [a,b]} |f^{(2)}(x)| = \max_{x \in [1,2]} \left| \frac{24}{x^5} \right| = 24$$

Plugging all this into our error bound for Simpson's Rule gives us our answer:

$$UBE = \frac{b-a}{180} h^4 \max_{x \in [a,b]} |f^{(4)}(x)| = \frac{1}{180} \times 0.25^4 \times 24 \approx 7.74 \times 10^{-4}$$