Lecture 18

Integration: Composite Trapezoid Rule, Recursion, and Simpson's 1/3 Rule

Ashley Gannon

ISC3313 Fall 2021

The Composite Trapezoid Rule Continued

Let's think back to our formula

If $a = x_0$ and $b = x_n$, the total integration with the trapezoidal rule can be represented by

$$I = h\frac{f(x_0) + f(x_1)}{2} + h\frac{f(x_1) + f(x_2)}{2} + ... + h\frac{f(x_{n-1}) + f(x_n)}{2}$$

If we expand this a bit more we can see a pattern emerge

$$I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + h\frac{f(x_2)+f(x_3)}{2} + ... + h\frac{f(x_{n-2})+f(x_{n-1})}{2} + h\frac{f(x_{n-1})+f(x_n)}{2}$$

And we can rewrite this equation as

$$I = \frac{h}{2} * (f(x_0) + f(x_n)) + \frac{h}{2}\sum_{i=1}^{n-1} 2f(x_i)$$

Which simplifies to

$$I = \frac{h}{2} * (f(x_0) + f(x_n)) + h\sum_{i=1}^{n-1} f(x_i)$$

The Composite Trapezoid Rule Pseudocode

```
function takes in a, b, n
declare/define h = (b-a)/n;
declare/define sum = (h/2)*(f(a)+f(b));
declare/define xi = a+h;

loop over i = 1,...,n-1
   add h*f(xi) to sum
   update xi = xi +h;
```

Thinking about the error

Last time we talked a bit about forming the error for the composite trapezoid rule. Recall that the error for the composite trapezoidal rule can be obtained by summing the individual errors for each segment to give

$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i+1}^{n} f''(\xi_i)$$

Where $f''(x_i)$ is the second derivative at a point ξ located in segment i. This result can be simplified by estimating the mean or average value of the second derivative for the entire interval as

$$\bar{f}'' \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

Subbing this into our equation for E_t, we can approximate the error E_a

$$E_a = -\frac{(b-a)^3}{12n^2}\bar{f}''$$

Where $\bar{f}''$ is found the same was as in the case of the single application of the trapezoidal rule. Which was done by finding the function's second derivative analytically, $f''(x) = -400 + 4050x - 10800x^2 + 8000x^3$, to find $f''(\xi)$, and then taking the average value of the second derivative by computing

$$\bar{f}''(x) = \frac{\int_0^{0.8}(-400 + 4050x - 10800x^2 + 8000x^3)dx}{0.8-0} = -60$$

So how can we use this error to get a better result?

If we look at our function,

$$E_a = -\frac{(b-a)^3}{12n^2}(-60)$$

we notice that E_a is only dependent on n now that we have evaluated $\bar{f}''(x)$.

So how can we use this error to get a better result?

If we look at our function,

$$E_a = -\frac{(b-a)^3}{12n^2}(-60)$$

we notice that E_a is only dependent on n now that we have evaluated $\bar{f}''(x)$.

If we want to modify our code so that this error falls below a desired tolerance, we will do this by using *recursion*.

Recursion

- In computer science, *recursion* is a method of solving a problem where the solution depends on solutions to smaller instances of the same problem.

Recursion

- In computer science, *recursion* is a method of solving a problem where the solution depends on solutions to smaller instances of the same problem.
  - So for this problem, we will take smaller and smaller segment sizes (h) until our error is less than our specified tolerance.

$$-\frac{(b-a)^3}{12n^2}(-60) < tol$$

Recursion

- In computer science, *recursion* is a method of solving a problem where the solution depends on solutions to smaller instances of the same problem.
  - So for this problem, we will take smaller and smaller segment sizes (h) until our error is less than our specified tolerance.

$$-\frac{(b-a)^3}{12n^2}(-60) < tol$$

- Recursive problems call themselves from within their own code.

Recursion

- In computer science, *recursion* is a method of solving a problem where the solution depends on solutions to smaller instances of the same problem.
  - So for this problem, we will take smaller and smaller segment sizes (h) until our error is less than our specified tolerance.

$$-\frac{(b-a)^3}{12n^2}(-60) < tol$$

- Recursive problems call themselves from within their own code.
- The approach can be applied to many types of problems, and recursion is one of the central ideas of computer science.

Recursive Composite Trapezoid Rule Pseudocode

declare function that takes in a, b, n, $\bar{f}''$, tolerance

declare/define the error $-\frac{(b-a)^3}{12n^2} * \bar{f}''$

```
if error > tolerance
This is where recursion comes in
   redefine n, n = 2*n for example
   return function(a,b,n,f̄'', tol)

declare/define h = (b-a)/n;
declare/define sum = (h/2)*(f(a)+f(b));
declare/define xi = a+h;

loop over i = 1,...,n-1
   add h*f(xi) to sum
   update xi = xi +h;
```

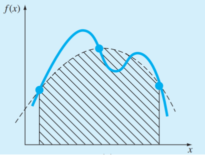
Simpson's Rules

Simpson's Rules

- Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points

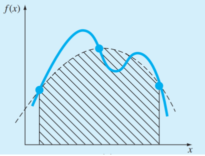
Simpson's Rules

- Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points
- For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola

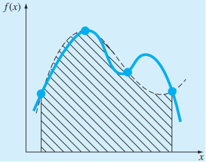


Simpson's Rules

- Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points
- For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola

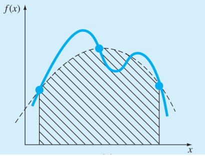


- If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial

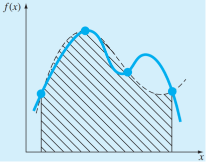


Simpson's Rules

- Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points
- For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola



- If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial



- The formulas that result from taking the integrals under these polynomials are called *Simpson's rules.*

Simpson's 1/3 Rule

Simpson's 1/3 Rule

Simpson's 1/3 rule corresponds to the case where the polynomial $f_n(x)$ in

$$I \cong \int_a^b f_n(x)dx$$

is

$$\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

Simpson's 1/3 Rule

Simpson's 1/3 rule corresponds to the case where the polynomial $f_n(x)$ in

$$I \cong \int_a^b f_n(x)dx$$

is

$$\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

Plugging this in and integrating from x_0 to x_2

$$I \cong \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)dx$$

Simpson's 1/3 Rule

Simpson's 1/3 rule corresponds to the case where the polynomial $f_n(x)$ in

$$I \cong \int_a^b f_n(x)dx$$

is

$$\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

Plugging this in and integrating from x_0 to x_2

$$I \cong \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)dx$$
$$= \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

Simpson's 1/3 Rule

Simpson's 1/3 rule corresponds to the case where the polynomial $f_n(x)$ in

$$I \cong \int_a^b f_n(x)dx$$

is

$$\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

Plugging this in and integrating from x_0 to x_2

$$I \cong \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)dx$$
$$= \frac{h}{3}(f(x_0) + 4F(x_1) + f(x_2))$$

Where $x_0 = a$, $x_2 = b$ and x_1 is their midpoint, $x_1 = \frac{a+b}{2}$. This is known as *Simpson's 1/3 Rule.*

Error in Simpson's 1/3 Rule

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Where ξ again lies somewhere on the interval from a to b. We evaluate this term the same was as before by finding the average of the fourth derivative.

$$\overline{f}^{(4)} = \frac{\int_a^b f^{(4)} dx}{b-a}$$

Error in Simpson's 1/3 Rule

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Where ξ again lies somewhere on the interval from a to b. We evaluate this term the same was as before by finding the average of the fourth derivative.

$$\bar{f}^{(4)} = \frac{\int_a^b f^{(4)} dx}{b-a}$$

- Simpson's 1/3 rule is more accurate than the trapezoidal rule.

Error in Simpson's 1/3 Rule

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Where ξ again lies somewhere on the interval from a to b. We evaluate this term the same was as before by finding the average of the fourth derivative.

$$\bar{f}^{(4)} = \frac{\int_a^b f^{(4)} dx}{b-a}$$

- Simpson's 1/3 rule is more accurate than the trapezoidal rule.
- The Trapezoid rule error was proportional to the second derivative, Simpson's 1/3 rule is proportional to the fourth derivative

Error in Simpson's 1/3 Rule

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Where ξ again lies somewhere on the interval from a to b. We evaluate this term the same was as before by finding the average of the fourth derivative.

$$\bar{f}^{(4)} = \frac{\int_a^b f^{(4)} dx}{b-a}$$

- Simpson's 1/3 rule is more accurate than the trapezoidal rule.
- The Trapezoid rule error was proportional to the second derivative, Simpson's 1/3 rule is proportional to the fourth derivative
- Simpson's 1/3 rule is third order accurate and yields exact results for cubic polynomials even though it is derived from a parabola

Single Application of Simpson's 1/3 Rule

Let's use a single application of Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recalling our formula for Simpson's 1/3 rule is

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

Single Application of Simpson's 1/3 Rule

Let's use a single application of Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recalling our formula for Simpson's 1/3 rule is

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

The first thing we need to do is calculate the value for x_1

$$x_1 = \frac{0.8 + 0}{2} = 0.4$$

Single Application of Simpson's 1/3 Rule

Let's use a single application of Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recalling our formula for Simpson's 1/3 rule is

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

The first thing we need to do is calculate the value for x_1

$$x_1 = \frac{0.8 + 0}{2} = 0.4$$

We can plug in the values for $h = \frac{0.8-0}{2}$, $f(0) = 0.2$, $f(0.4) = 2.456$, and $f(0.8) = 0.232$

$$I = \frac{0.8 - 0}{2 * 3}(0.2 + 4(2.456) + 0.232) = 1.367467$$

Error in A Single Application of Simpson's 1/3 Rule

Recalling our error formula

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Error in A Single Application of Simpson's 1/3 Rule

Recalling our error formula

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

We need to first evaluate $f^{(4)}(\xi)$ by finding the average of the fourth derivative.

$$f^{(4)} = 48000x - 21600$$

Error in A Single Application of Simpson's 1/3 Rule

Recalling our error formula

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

We need to first evaluate $f^{(4)}(\xi)$ by finding the average of the fourth derivative.

$$f^{(4)} = 48000x - 21600$$

To find the average

$$\begin{aligned}\bar{f}^{(4)}(x) &= \frac{\int_a^b f^{(4)}(x)dx}{b-a} \\ &= \frac{\int_0^{0.8}(48000x - 21600)dx}{0.8-0} \\ &= -2400\end{aligned}$$

Error in A Single Application of Simpson's 1/3 Rule

Recalling our error formula

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

We need to first evaluate $f^{(4)}(\xi)$ by finding the average of the fourth derivative.

$$f^{(4)} = 48000x - 21600$$

To find the average

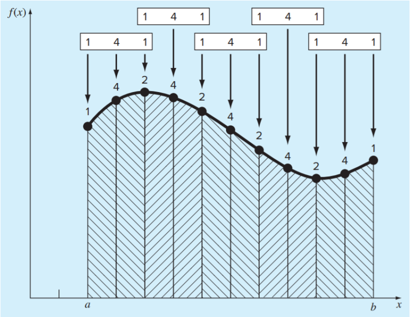
$$\begin{aligned}\bar{f}^{(4)}(x) &= \frac{\int_a^b f^{(4)}(x)dx}{b-a} \\ &= \frac{\int_0^{0.8}(48000x - 21600)dx}{0.8-0} \\ &= -2400\end{aligned}$$

Plugging this into our error we have

$$E_a = -\frac{(0.8-0)^5}{2880}(-2400) = 0.2730667$$

Composite Simpson's 1/3 Rule

Just as with the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width.



The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{n-2}}^{x_n} f(x)dx$$

Composite Simpson's 1/3 Rule

The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{n-2}}^{x_n} f(x)dx$$

Composite Simpson's 1/3 Rule

The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{n-2}}^{x_n} f(x)dx$$

Substituting Simpson's 1/3 rule for each integral yields

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4))$$
$$+ ... + \frac{h}{3}(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n))$$

Composite Simpson's 1/3 Rule

The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{n-2}}^{x_n} f(x)dx$$

Substituting Simpson's 1/3 rule for each integral yields

$$\begin{aligned} I = &\frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4)) \\ &+ ... + \frac{h}{3}(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)) \end{aligned}$$

Which can be re-written using summation notation

$$I = \frac{h}{3}(f(x_0) + f(x_n)) + \frac{h}{3}\left(4 \sum_{i=1,3,5\dots}^{n-1} f(x_i) + 2 \sum_{j=2,4,6,\dots}^{n-2} f(x_j)\right)$$

Composite Simpson's 1/3 Rule

The total integration can be represented as

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{n-2}}^{x_n} f(x)dx$$

Substituting Simpson's 1/3 rule for each integral yields

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4))$$
$$+ ... + \frac{h}{3}(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n))$$

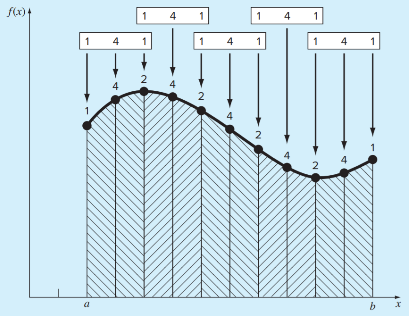
Which can be re-written using summation notation

$$I = \frac{h}{3}(f(x_0) + f(x_n)) + \frac{h}{3}\left(4 \sum_{i=1,3,5\ldots}^{n-1} f(x_i) + 2 \sum_{j=2,4,6,\ldots}^{n-2} f(x_j)\right)$$

The coefficients 4 and 2 in might seem peculiar at first glance. However, they follow naturally from Simpson's 1/3 rule, as illustrated in the previous/following image.

Composite Simpson's 1/3 Rule

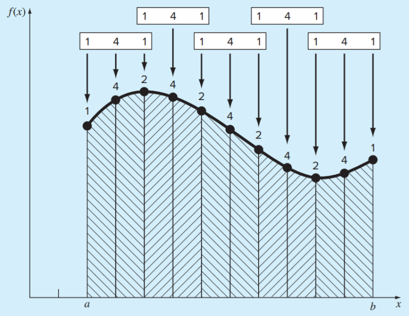
If we look back at the diagram for composite Simpson's 1/3 rule,



- we notice that we must have an even number of segments to implement this method.

Composite Simpson's 1/3 Rule

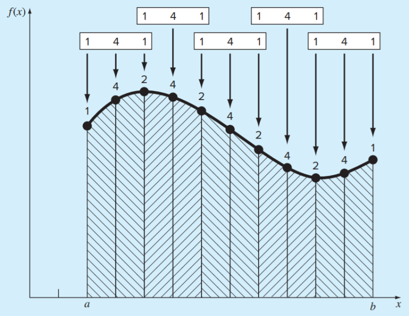
If we look back at the diagram for composite Simpson's 1/3 rule,



- we notice that we must have an even number of segments to implement this method.
- We also can see from this figure that the odd points represent the middle term for each application which carry a weight of 4.

Composite Simpson's 1/3 Rule

If we look back at the diagram for composite Simpson's 1/3 rule,



- we notice that we must have an even number of segments to implement this method.
- We also can see from this figure that the odd points represent the middle term for each application which carry a weight of 4.
- And also that the even points are common to adjacent applications and are counted twice.

Error in Composite Simpson's 1/3 Rule

An error estimate for the composite Simpson's rule is obtained in the same fashion as for the trapezoidal rule by summing the individual errors for the segments and averaging the derivative to yield

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)}$$

where $f^{(4)}$ is the average fourth derivative for the interval.

Composite Simpson's 1/3 Rule Example

Let's use the composite Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$, and $n = 4$.

We first need to compute our h,

$$h = \frac{0.8 - 0}{4} = 0.2$$

Composite Simpson's 1/3 Rule Example

Let's use the composite Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$, and $n = 4$.

We first need to compute our h,

$$h = \frac{0.8 - 0}{4} = 0.2$$

now we can compute our values for x_1, x_2, and x_3

$$x_1 = a + h = 0.2$$

$$x_2 = x_1 + h = 0.4$$

$$x_3 = x_2 + h = 0.6$$

Composite Simpson's 1/3 Rule Example

Let's use the composite Simpson's 1/3 rule to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$, and $n = 4$.

We first need to compute our h,

$$h = \frac{0.8 - 0}{4} = 0.2$$

now we can compute our values for x_1, x_2, and x_3

$$x_1 = a + h = 0.2$$

$$x_2 = x_1 + h = 0.4$$

$$x_3 = x_2 + h = 0.6$$

And plug these values into f

$$f(0) = 0.2$$

$$f(0.2) = 1.288$$

$$f(0.4) = 2.456$$

$$f(0.6) = 3.464$$

$$f(0.8) = 0.232$$

Composite Simpson's 1/3 Rule Example

Substituting these values into our equation

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4))$$

We get

$$I = \frac{0.8}{12}(0.2 + 4(0.2) + 2(2.456) + 2(3.464) + 0.232) = 1.623467$$

.

Composite Simpson's 1/3 Rule Example

Substituting these values into our equation

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4))$$

We get

$$I = \frac{0.8}{12}(0.2 + 4(0.2) + 2(2.456) + 2(3.464) + 0.232) = 1.623467$$

Which has an approximate error of

$$E_a = -\frac{(b-a)^5}{180(4)^4}(-2400) = 0.017067$$

which is 80% less than the single application.

Exercise

How would you code the composite Simpson's 1/3 rule? Write your pseudocode and submit it to the canvas discussion board **Composite Simpson's 1/3 Rule**.

NOTE: Use recursion to find the n that drives the error to be less than your tolerance.