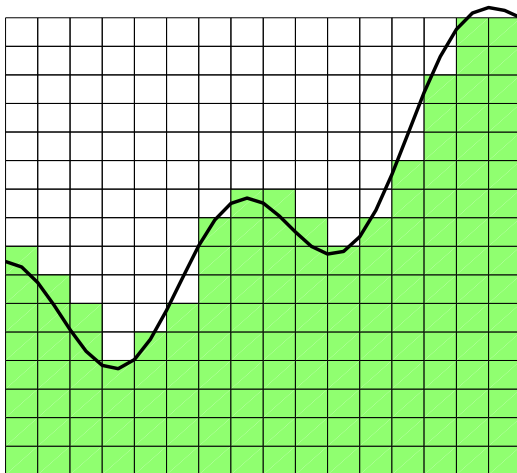


$$\int_a^b f(x) dx$$



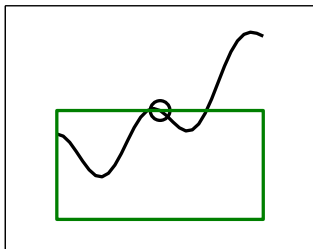
**Adaptive Quadrature**

$$\int_a^b f(x) dx = \int_a^c f(x) dx + \int_c^b f(x) dx$$

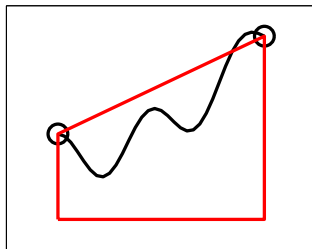
## Midpoint and Trapezoid Rules

$$M = hf\left(\frac{a+b}{2}\right)$$
$$T = h\frac{f(a) + f(b)}{2}$$

Midpoint rule



Trapezoid rule



Both are *exact* for linear functions (polynomials of degree 1).

## Example

$$\int_0^1 x^2 dx = \frac{1}{3}$$

$$M = 1 \left( \frac{1}{2} \right)^2 = \frac{1}{4}$$

$$T = 1 \frac{0 + 1^2}{2} = \frac{1}{2}$$

$$\begin{aligned}I &= \int_0^1 x^2 dx = \frac{1}{3}, & M &= \frac{1}{4}, & T &= \frac{1}{2} \\I - T &= -\frac{1}{6}, & I - M &= \frac{1}{12} \\I - T &= -2(I - M)\end{aligned}$$

This is actually (approximately) true in general. The error in the trapezoid rule is about twice as big as that in the midpoint rule (and with reversed sign).

### Error Analysis

First a definition.

#### Definition

We say that a quadrature method has order  $p$  if it is exact for polynomials of degree  $p - 1$  or less.

#### Example

Both the midpoint rule and the trapezoid rule are order two rules, since they are exact for polynomials of degree one.

If a quadrature rule is order  $p$ , then the error in the approximation is

$$\mathcal{O}(h^p)$$

The main tool of error analysis is Taylor's theorem:

### Taylor's Theorem

$$f(x) = f(a) + f'(a)(x - a) + \frac{1}{2}f''(a)(x - a)^2 + \cdots + \frac{1}{n!}f^{(n)}(a)(x - a)^n \\ + \frac{1}{(n+1)!}f^{(n+1)}(\xi)(x - a)^{n+1}$$

for some  $\xi$  between  $a$  and  $x$ .

This is often written using  $h = x - a$  as

$$f(a + h) = f(a) + hf'(a) + \frac{h^2}{2}f''(a) + \frac{h^3}{3!}f'''(a) + \cdots + \frac{h^n}{n!}f^{(n)}(a) + \frac{h^{n+1}}{(n+1)!}f^{(n+1)}(\xi)$$

## Trapezoid Rule

For the trapezoid rule, we have, using  $h = b - a$  in Taylor's Theorem

$$\begin{aligned} I &= \int_a^b f(x) dx \\ T &= \frac{h}{2}(f(a) + f(b)) \\ &= \frac{h}{2}(f(a) + f(a+h)) \\ &= \frac{h}{2} \left( f(a) + f(a) + hf'(a) + \frac{h^2}{2}f''(c) \right) \\ &= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{4}f''(c) \end{aligned}$$

for some  $c$  between  $a$  and  $b$ .



Now write

$$F(t) = \int_a^{a+t} f(x) dx$$

By the Fundamental Theorem of Calculus,  $F'(x) = f(x)$ , and by Taylor's Theorem,

$$\begin{aligned} I &= F(h) \\ &= F(0) + hF'(0) + \frac{h^2}{2}F''(0) + \frac{h^3}{3!}F'''(d) \\ &= 0 + hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(d) \end{aligned}$$

for some  $d$  between  $a$  and  $b$ . Now, since

$$T = hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{4}f''(c)$$

$$T - I = \frac{h^3}{12}f''(\xi)$$

## Midpoint Rule

For the midpoint rule, we have

$$\begin{aligned}M &= hf\left(\frac{a+b}{2}\right) \\&= hf\left(a + \frac{h}{2}\right) \\&= h\left(f(a) + \frac{h}{2}f'(a) + \frac{1}{2}\left(\frac{h}{2}\right)^2 f''(e)\right) \\&= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{8}f''(e)\end{aligned}$$

Comparing with what we got for the exact integral  $I$ , we see

$$M - I = -\frac{h^3}{24}f''(\zeta)$$

Perhaps surprisingly, the midpoint rule is more accurate than the trapezoid rule.

$$T - I = \frac{h^3}{12} f''(\xi) \quad \text{and} \quad M - I = -\frac{h^3}{24} f''(\zeta)$$

Therefore

$$T - I \approx -2(M - I)$$

## Composite Trapezoid Rule

Of course we don't want just one interval. Break the interval  $(a, b)$  up into  $n$  sub-intervals

$$a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$$

Let

$$h_i = x_{i+1} - x_i$$

Then the composite trapezoid rule is

$$T_n = \sum_{i=1}^n \frac{h_i}{2} (f(x_{i-1}) + f(x_i))$$

If the subintervals are equally spaced,

$$h_i = h = \frac{b-a}{n}$$

then the error on each subinterval is  $\mathcal{O}(h^3)$ . There are  $n = \frac{b-a}{h}$  subintervals, so the **total error** is

$$E_T = \mathcal{O}(h^2)$$

The total error in the trapezoidal rule is

$$E_T = \mathcal{O}(h^2)$$

This is another sense in which the method is order two. Doubling the number of intervals reduces the error by (roughly) half.

The composite trapezoidal method is implemented in Matlab as

```
trapz(x,y)
```

## Simpson's Rule

Since we have

$$T - I \approx -2(M - I)$$

we can get a better approximation by combining the midpoint and trapezoid rules. Call  $S$  our approximation and determine  $S$  as the solution of the above if it was an equation, i.e.

$$T - S = -2(M - S)$$

Solving for  $S$  gives us

$$S = \frac{T + 2M}{3}$$

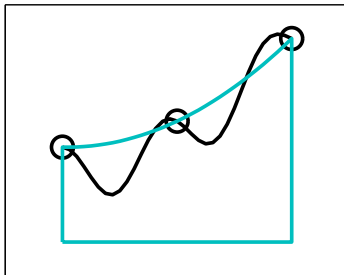
Let  $c = \frac{a+b}{2}$ . Then

$$S = \frac{h}{6} (f(a) + 4f(c) + f(b))$$

This is known as *Simpson's Rule*.

$$S = \frac{h}{6} (f(a) + 4f(c) + f(b))$$

**Simpson's rule**





## Error Analysis of Simpson's Rule

We use Taylor's Theorem again:

$$\begin{aligned}
 S &= \frac{h}{6} [f(a) + 4f(c) + f(b)] \\
 &= \frac{h}{6} \left[ f(a) + 4f\left(a + \frac{h}{2}\right) + f(a+h) \right] \\
 &= \frac{h}{6} \left[ f(a) + 4 \left( f(a) + \frac{h}{2} f'(a) + \frac{h^2}{8} f''(a) + \frac{h^3}{48} f'''(a) + \frac{h^4}{16 \cdot 24} f^{(4)}(d) \right) \right. \\
 &\quad \left. + f(a) + hf'(a) + \frac{h^2}{2} f''(a) + \frac{h^3}{6} f'''(a) + \frac{h^4}{24} f^{(4)}(e) \right] \\
 &= hf(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{6} f''(a) + \frac{h^4}{24} f'''(a) + \frac{5h^5}{576} f^{(4)}(\xi)
 \end{aligned}$$

As before we write

$$F(t) = \int_a^{a+t} f(x) dx$$

So the exact integral is

$$\begin{aligned} I &= F(h) \\ &= F(0) + hF'(0) + \frac{h^2}{2}F''(0) + \frac{h^3}{3!}F'''(0) + \frac{h^4}{4!}F^{(4)}(0) + \frac{h^5}{5!}F^{(5)}(\alpha) \\ &= 0 + hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \frac{h^4}{24}f'''(a) + \frac{h^5}{120}f^{(4)}(\alpha) \end{aligned}$$

Compare these two:

$$S = hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \frac{h^4}{24}f'''(a) + \frac{5h^5}{576}f^{(4)}(\xi)$$

$$I = hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \frac{h^4}{24}f'''(a) + \frac{h^5}{120}f^{(4)}(\alpha)$$

They agree up to the fourth term! This means that Simpson's Rule is actually order 4! It is exact for cubic polynomials.

$$S - I = \frac{h^5}{24 \cdot 5!} f^{(4)}(\zeta)$$

The error in each interval is

$$\mathcal{O}(h^5)$$

Composite Simpson's:

$$S_n = \frac{h}{6} \sum_{i=1}^{n/2} [f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})], \quad h = \frac{b-a}{2n}$$

The total error is

$$E_T = \mathcal{O}(h^4)$$

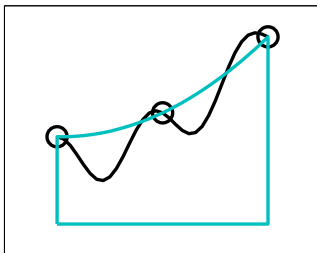
A reduction of the step size by one-half reduces the error by  $\frac{1}{16}$ .

## Adaptive Simpson's

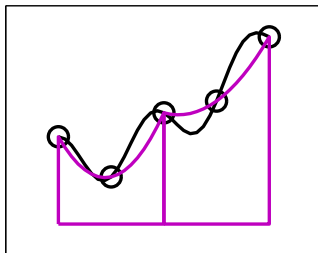
$$S = \frac{h}{6} (f(a) + 4f(c) + f(b))$$

$$S_2 = \frac{h}{12} (f(a) + 4f(d) + 2f(c) + 4f(e) + f(b))$$

Simpson's rule



Composite Simpson's rule



Approximate error:

$$E = S_2 - S$$

Adaptive algorithm:

```
if |S2 - S| < tol
  use these quantities to get a good approximation
else
  divide intervals by 2 and start again to the left
end
```

Each approximation on a subinterval has error of order

$$\left(\frac{h}{2}\right)^5$$

so the error in  $S_2$  is approximately

$$\frac{1}{2}2^5 = 2^4 = 16$$

times as good as  $S$ . That is, the exact value  $I$  is approximately

$$I - S \approx 16(I - S_2)$$

That is to say,

$$I \approx S_2 + \frac{S_2 - S}{15}$$

We use this after calculating  $S$  and  $S_2$  to obtain our approximation.