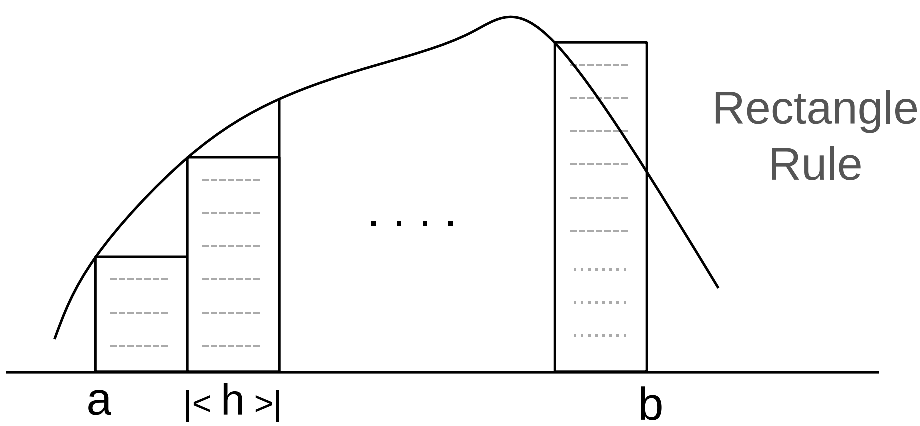
Numerical Integration

Introduction There are two types of integrals: indefinite integral and definite integral. If we can find an anti-derivative $F(x)$ of a function f, and F is an elementary function, then we can compute

$$I = \int_a^b f(x)dx = F(b) - F(a).$$

Maple and Mathematica **can** do **symbolic integration** (when possible).
However often it is **not possible** to obtain such an $F(x)$ for $f(x)$. e.g. the case of $f(x) = e^{-x^2}$. When symbolic integration is not feasible, we can use **numerical integration**, to **approximate** an integral by something which is **much easier to compute**.
One important interpretation for the definite integral $\int_a^b f(x)dx$ is it is the **area** between the graph of f and the x-axis on this interval (here the area may be negative).

Rectangle Rule



Partition $[a, b]$ into n equal subintervals $[x_i, x_{i+1}]$, $i = 0, 1, \ldots, n-1$, all with width $h = (b-a)/n$. Each rectangle touches the graph of f at its top left corner.
The area of the rectangle over $[x_i, x_{i+1}]$ is

$$hf(x_i) = hf(a + ih).$$

The **total area** of the n rectangle panels is

$$I_R = h\sum_{i=0}^{n-1} f(a + ih).$$

This is an approximation of $I = \int_a^b f(x)dx$ and it is called the (left composite) **rectangle rule** (for n equal subintervals). Note that f is evaluated at n discrete points.

Error Analysis of the Rectangle Rule

Tools for error analysis: The Mean-Value-Theorem

- for sum: Let $q(x)$ be continuous on $[a,b]$. If $p(z_i) \geq 0$ for $i = 1, \ldots, n$, then
$$\sum_{i=1}^{n} p(z_i)q(z_i) = q(z)\sum_{i=1}^{n} p(z_i), \quad \text{some } z \in [a,b],$$
- for integrals: Let $q(x)$ and $p(x)$ be continuous with $p(x) \geq 0$. Then
$$\int_a^b p(x)q(x)dx = q(z)\int_a^b p(x)dx, \text{ some } z \in [a,b]$$

Theorem: Let f' be continuous on $[a,b]$. Then for some $z \in [a,b]$,
$$I - I_R = \frac{1}{2}(b-a)hf'(z) = O(h).$$

Proof: We first show when $h = b-a$, it is true, i.e.,
$$I - I_R = \frac{1}{2}(b-a)^2 f'(z), \text{ for some } z \in [a,b] \quad (*)$$

For every $x \in [a,b]$, the Taylor series expansion gives
$$f(x) = f(a) + (x-a)f'(z_x), \quad \text{for some } z_x \in [a,b].$$

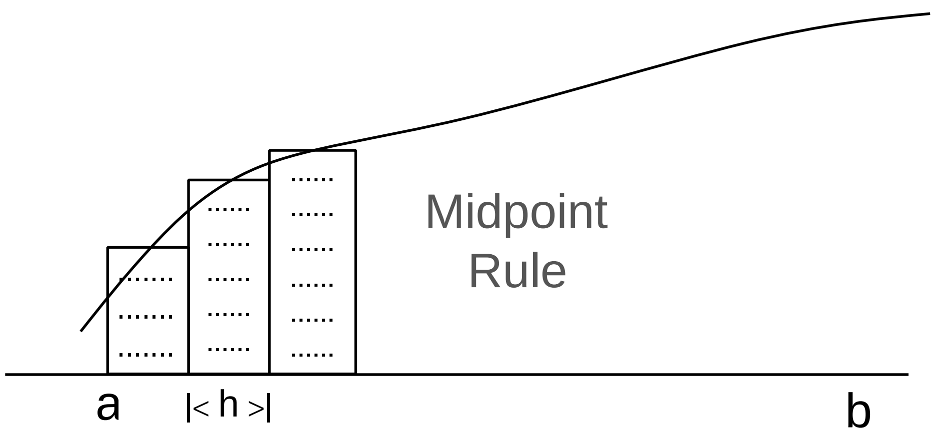
Then
$$\begin{aligned} I - I_R &= \int_a^b f(x)dx - f(a)(b-a) \\ &= \int_a^b f(x)dx - \int_a^b f(a)dx \\ &= \int_a^b [f(x) - f(a)]dx \\ &= \int_a^b (x-a)f'(z_x)dx \\ &= f'(z)\int_a^b (x-a)dx \quad \text{(MVT for integral)} \\ &= \frac{1}{2}(b-a)^2 f'(z). \end{aligned}$$

Now let $[a,b]$ be divided into n equal subintervals by $x_0, x_1, \ldots, x_n$ with spacing $h = (b-a)/n$. Applying $(*)$ to subinterval $[x_i, x_{i+1}]$, we have
$$\int_{x_i}^{x_{i+1}} f(x)dx - f(x_i)h = \frac{(x_{i+1}-x_i)^2}{2}f'(z_i) = \frac{h^2}{2}f'(z_i),$$

for some $z_i \in [x_i, x_{i+1}]$. So we have

$$\begin{aligned}
I - I_R &= \int_a^b f(x)dx - h\sum_{i=0}^{n-1} f(x_i) \\
&= \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx - h\sum_{i=0}^{n-1} f(x_i) \\
&= \sum_{i=0}^{n-1}\frac{1}{2}h^2\cdot f'(z_i) \\
&= f'(z)\cdot\frac{1}{2}nh^2 \qquad \text{(MVT for sum)} \\
&= \frac{1}{2}(b-a)hf'(z).
\end{aligned}$$

Midpoint Rule



,

We make the **midpoint** of the top of each rectangle intersect the graph.
The midpoint rule:

$$I_M = h\sum_{i=0}^{n-1} f[a+(i+1/2)h], \quad \text{where } h = \frac{b-a}{n}.$$

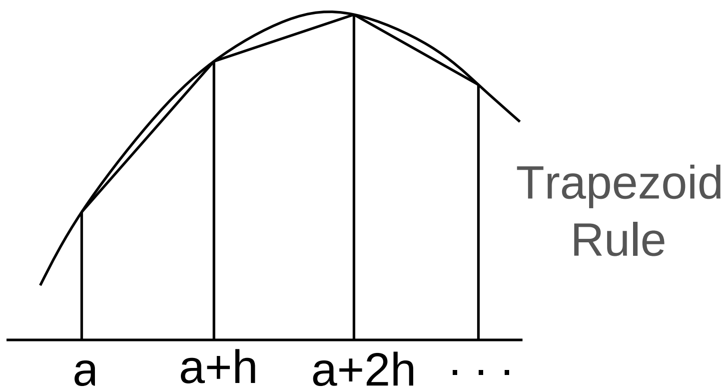
Since **part** of the rectangle usually lies **above** the graph of f and **part below**, the midpoint rule is **more accurate** than the rectangle rule.
It can be proven that for some $z \in [a, b]$

$$I - I_M = \frac{1}{24}(b-a)h^2f''(z) = O(h^2).$$

(Try to prove it by yourself)

Trapezoid Rule

Consider **trapezoid-shaped panels**:



The trapezoid rule:

$$I_T = \frac{1}{2}h[f(a) + f(b)] + h\sum_{i=1}^{n-1} f(a+ih), \text{ with } h = \frac{b-a}{n}.$$

It can be shown that for some $z \in [a, b]$

$$I - I_T = -\frac{1}{12}(b-a)h^2 f''(z) = O(h^2).$$

Q Prove both the midpoint and trapezoid rules give the **exact** integral if f is **linear**.

Recursive Trapezoid Rule

Suppose $[a, b]$ is divided into 2^n equal subintervals. Then the trapezoid rule is

$$I_T(2^n) = \frac{1}{2}h[f(a) + f(b)] + h\sum_{i=1}^{2^n-1} f(a+ih).$$

where $h = (b-a)/2^n$.
The trapezoid rule for 2^{n-1} equal subintervals is

$$I_T(2^{n-1}) = \frac{1}{2}\tilde{h}[f(a) + f(b)] + \tilde{h}\sum_{i=1}^{2^{n-1}-1} f(a+i\tilde{h}).$$

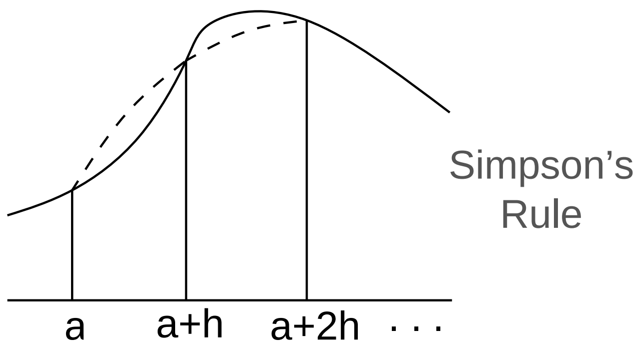
where $\tilde{h} = (b-a)/2^{n-1} = 2h$. It is easy to show the following recursive formula

$$I_T(2^n) = \frac{1}{2} I_T(2^{n-1}) + h \sum_{i=1}^{2^{n-1}} f[a + (2i-1)h].$$

After computing $I_T(2^{n-1})$ we can compute $I_T(2^n)$ by this recursive formula without reevaluating f at the old points.

Simpson's Rule

There is no need for straight edges:



Each panel is topped by a **parabola**.
There are an **even** number of panels with width $h = (b-a)/n$. The top boundary of the first pair of panels is **the quadratic which interpolates** $(a, f(a))$, $(a+h, f(a+h))$, $(a+2h, f(a+2h))$. The next interpolates $(a+2h, f(a+2h))$, $(a+3h, f(a+3h))$, $(a+4h, f(a+4h))$, and so on.
The area of the first 2 panels can be shown to be

$$\frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right]$$

Q: How would you obtain this **??**
Summing the areas of the pairs

$$\frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)],$$

$$\frac{h}{3}[f(a+2h) + 4f(a+3h) + f(a+4h)],$$

$$\cdots\cdots\cdots$$

$$\frac{h}{3}[f(b-2h) + 4f(b-h) + f(b)],$$

leads to **Simpson's rule** ($h = \frac{b-a}{n}$):

$$I_S = \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots$$
$$+4f(b-3h) + 2f(b-2h) + 4f(b-h) + f(b)].$$

It can be shown for some $z \in [a, b]$

$$I - I_S = -\frac{1}{180}(b-a)h^4 f^{(4)}(z) = O(h^4).$$

Q: What is the highest degree polynomial for which the rule is **exact** in general **??**

Adaptive Simpson's Method

Motivation and ideas of an adaptive integration method:
A function may varies rapidly on some parts of the interval $[a, b]$, but varies little on other parts. It is not very efficient to use some panel width h everywhere on $[a, b]$. But on the other hand, it is not known in advance on which part of the integral f varies rapidly. We can consider an adaptive integration method. The basic idea is we divide $[a, b]$ into 2 subintervals and then decide whether each of them is to be divided into more subintervals. This procedure is continued until some specified accuracy is obtained throughout the whole interval $[a, b]$.

A framework of an adaptive method:

function $numI = adapt(f, a, b, \epsilon, \cdots)$
  Compute the integral from a and b in two ways
  and call the values I_1 and I_2 (assume I_2 is better than I_1)
  Estimate the error in I_2 based on $|I_2 - I_1|$
  if |the estimated error| $\leq \epsilon$, then
    $numI = I_2$ (or $numI = I_2 +$ the estimated error)
  else
    $c = (a+b)/2$
    $numI = adapt(f, a, c, \epsilon/2, \cdots)$
        $+adapt(f, c, b, \epsilon/2, \cdots)$
  end

This will guarantee $|I - numI| \lesssim \epsilon$.
Now we want to fill in details for Simpson's method.

- Defining I_1 and I_2:
  Simpson's rule for $n = 2$ gives
  $$I = I_1 + E_1,$$
  where
  $$I_1 = \frac{b-a}{6}[f(a) + 4f(\frac{a+b}{2}) + f(b)],$$
  $$E_1 = -\frac{1}{180}(b-a)(\frac{b-a}{2})^4 f^{(4)}(z).$$
  Simpson's rule for $n = 4$ gives
  $$I = I_2 + E_2,$$
  where
  $$I_2 = \frac{b-a}{12}[f(a) + 4f(a + \frac{b-a}{4})$$
  $$+2f(a + \frac{b-a}{2}) + 4f(a + \frac{3(b-a)}{4}) + f(b)],$$
  $$E_2 = -\frac{1}{180}(b-a)(\frac{b-a}{4})^4 f^{(4)}(\tilde{z}).$$
- Estimating the error in I_2:
  We assume $f^{(4)}(z)$ in E_1 is equal to $f^4(\tilde{z})$ in E_2. (a reasonable assumption if $f^{(4)}$ does not vary much on $[a, b]$). Then we observe
  $$E_1 = 16E_2.$$
  Since $I = I_1 + E_1 = I_2 + E_2$, we have
  $$I_2 - I_1 = E_1 - E_2 = 16E_2 - E_2 = 15E_2.$$
  This gives an error estimate in I_2:
  $$E_2 = \frac{1}{15}(I_2 - I_1).$$

Adaptive Simpson's algorithm:

function $numI = adapt\_simpson(f, a, b, \epsilon, level, level\_max)$

$h \leftarrow b - a$

$c \leftarrow (a + b)/2$

$I_1 \leftarrow h[f(a) + 4f(c) + f(b)]/6$

$level \leftarrow level + 1$

$d \leftarrow (a + c)/2$

$e \leftarrow (c + b)/2$

$I_2 \leftarrow h[f(a) + 4f(d) + 2f(c) + 4f(e) + f(b)]/12$

if $level \geq level\_max$, then

$numI \leftarrow I_2$

else

if $|I_2 - I_1| \leq 15\epsilon$, then

$numI \leftarrow I_2$ (or $numI \leftarrow I_2 + \frac{1}{15}(I_2 - I_1)$)

else

$$numI \leftarrow adapt\_simpson(f, a, c, \epsilon/2, level, level\_max) + adapt\_simpson(f, c, b, \epsilon/2, level, level\_max)$$

end

end

Gaussian Quadrature Rules

Unlike previous (composite) integration rules which choose equally spaced nodes for evaluation, Gaussian quadratiure rules choose the nodes $x_0, x_1, \ldots, x_n$ and coefficients $A_0, A_1, \ldots, A_n$ (which are also called weights) to minimize the expected error obtained in the approximation

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

To measure this accuracy, we assume that the best choice of these values is that which produces the exact result for the largest class of polynomials.

Theorem. Let q be a nontrival polynomial of degree $n+1$ such that

$$\int_a^b x^k q(x)dx = 0, \qquad k = 0, 1, \ldots, n. \tag{1}$$

Let $x_0, x_1, \ldots, x_n$ be the zeros of q. Then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} A_i f(x_i), \quad A_i = \int_a^b l_i(x)dx, \quad l_i(x) = \Pi_{j=0, j\neq i}^{n}\left(\frac{x - x_j}{x_i - x_j}\right),$$

for any polynomial $f(x)$ with degree less than or equal to $2n+1$.

Any $I_G = \sum_{i=0}^{n} A_i f(x_i)$ with x_i and A_i $(i = 0, 1, \ldots n)$ defined as in the above theorem called a Gaussian quadrature rule.

If the interval $[a, b] = [-1, 1]$, the Legendre polynomial $q_{n+1}(x)$ defined by

$$q_{n+1}(x) = \frac{2n+1}{n+1} x q_n(x) - \frac{n}{n+1} q_{n-1}(x), \quad q_0(x) = 1, \quad q_1(x) = x.$$

satisfies (1). Thus the roots of $q_{n+1}(x) = 0$ are the nodes of the Gaussian quadrature rule for $\int_{-1}^{1} f(x)dx$.

If the Gaussian quadrature rule for $\int_{-1}^{1} f(x)dx$ is $I_G[-1, 1] = \sum_{i=0}^{n} A_i f(x_i)$. Then it can shown that the Gaussian quadrature rule for $\int_a^b f(x)dx$ is

$$I_G[a, b] = \beta \sum_{i=0}^{n} A_i f(\alpha + \beta x_i), \quad \alpha = \frac{1}{2}(a+b), \quad \beta = \frac{1}{2}(b-a).$$