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
  \[
  \sum_{i=1}^{n} p(z_i)q(z_i) = q(z) \sum_{i=1}^{n} p(z_i), \text{ some } z \in [a, b],
  \]

- 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.,
\[
I - I_R = \frac{1}{2}(b-a)^2 f'(z), \text{ for some } z \in [a, b] \quad (\ast)
\]
For every \( x \in [a, b] \), the Taylor series expansion gives
\[
f(x) = f(a) + (x-a)f'(z_x), \text{ for some } z_x \in [a, b].
\]
Then
\[
I - I_R = \int_{a}^{b} f(x)dx - f(a)(b-a)
= \int_{a}^{b} f(x)dx - \int_{a}^{b} f(a)dx
= \int_{a}^{b} [f(x) - f(a)]dx
= \int_{a}^{b} (x-a)f'(z_x)dx
= f'(z) \int_{a}^{b} (x-a)dx \quad \text{(MVT for integral)}
= \frac{1}{2}(b-a)^2 f'(z).
\]

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 \((\ast)\) 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

$$I - I_R = \int_a^b f(x)dx - h \sum_{i=0}^{n-1} f(x_i)$$

$$= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx - h \sum_{i=0}^{n-1} f(x_i)$$

$$= \sum_{i=0}^{n-1} \frac{1}{2} h^2 \cdot f'(z_i)$$

$$= f'(z) \cdot \frac{1}{2} nh^2 \quad \text{(MVT for sum)}$$

$$= \frac{1}{2} (b - a) hf'(z).$$

**Midpoint Rule**

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

**The midpoint rule:**

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

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 $z \in [a, b]$

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

(Try to prove it by yourself)
Consider **trapezoid-shaped panels**:

![Trapezoid Rule Diagram](image)

The trapezoid rule:

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

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

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

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

Q: How would you obtain this ??

Summing the areas of the pairs

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

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

\[ \ldots \ldots \ldots \]

\[
\frac{h}{3} [f(b - 2h) + 4f(b - h) + f(b)],
\]
leads to **Simpson’s rule** \((h = \frac{b-a}{n})\):

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

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 \(|\text{the estimated error}| \leq \epsilon\)
    then
        \(numI = I_2\) \ (or \(numI = I_2 + \text{the estimated error}\))
    else
        \(c = \frac{(a + b)}{2}\)
        \(numI = adapt(f, a, c, \epsilon/2, \cdots) + adapt(f, c, b, \epsilon/2, \cdots)\)
    end

This will guarantee \(|I - numI| \leq \epsilon\).

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

$$I_1 = \frac{b - a}{6} [f(a) + 4f\left(\frac{a + b}{2}\right) + f(b)],$$

$$E_1 = -\frac{1}{180} (b - a)(\frac{b - a}{2})^4 f^{(4)}(z).$$

Simpson’s rule for $n = 4$ gives

$$I = I_2 + E_2,$$

where

$$I_2 = \frac{b - a}{12} \left[ f(a) + 4f\left(a + \frac{b - a}{4}\right) + 2f\left(a + \frac{b - a}{2}\right) + 4f\left(a + \frac{3(b - a)}{4}\right) + f(b) \right],$$

$$E_2 = -\frac{1}{180} (b - a)(\frac{b - a}{4})^4 f^{(4)}(\tilde{z}).$$

• 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
end
Gaussian Quadrature Rules

Unlike previous (composite) integration rules which choose equally spaced nodes for evaluation, Gaussian quadrature 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 nontrivial polynomial of degree $n+1$ such that

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

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

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

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

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