Numerical Integration

(Reading: Cheney and Kincaid, §5.1, §5.3, §5.4)

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

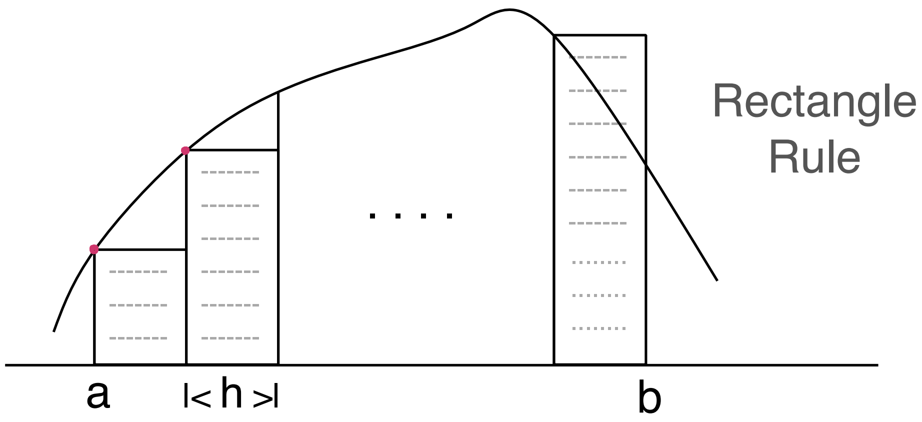
$$I = \int_a^b f(x)dx = F(b) - F(a).$$

general formula for F

Maple, Mathematica and MATLAB's Symbolic Math Toolbox **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**. sought at a particular input or set of inputs.

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). This can be used to develop some numerical methods.

Rectangle Rule



Partition $[a, b]$ into n equal subintervals $[x_i, x_{i+1}]$, $i = 0, 1, \ldots, n$, all with width $h = (b - a)/n$.

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 $z \in [a,b]$,

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

Given error tolerence compute n

Proof: We first show that when $h = b - a$ the result holds, i.e.,

$$I - I_R = \frac{1}{2}(b-a)^2 f'(z), \text{ for some } z \in [a,b]. \tag{1}$$

For any $x \in [a,b]$, the Taylor theorem gives

$$f(x) = f(a) + (x-a)f'(z_x), \text{ for some } z_x \in [a,b].$$

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 suppose $[a,b]$ is divided into n equal subintervals by $x_0, x_1, \ldots, x_n$ with panel width $h = (b-a)/n$. Applying the above result to the subinterval $[x_i, x_{i+1}]$, we have

$$\int_{x_i}^{x_{i+1}} f(x)dx - f(x_i)h = \frac{(x_{i+1}-x_i)^2}{2}f'(z_i) = \frac{h^2}{2}f'(z_i), \quad \text{for some } z_i \in [x_i, x_{i+1}].$$

So we have

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

□

The error formula not only helps us to understand the accuracy of the rectangle rule, but also can be used to determine h such that the error is bounded by a given tolerance. One example will be given in class.

$f(x)=x^2$, $tol = 10^{-6}$, $\int_0^1 f(x)dx$

$\frac{1}{2}(b-a)hf'(z) \le 10^{-6}$

$\uparrow$ 1 $\quad \uparrow$ $z \in [0,1]$

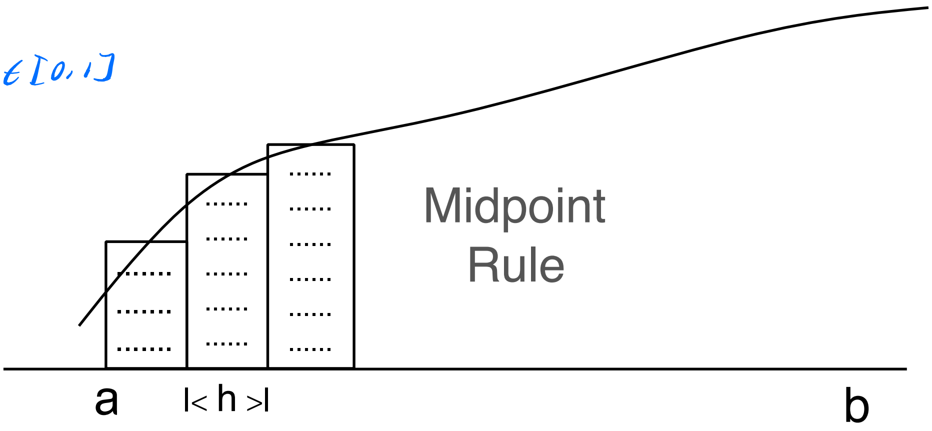
$h \le \frac{2\cdot 10^{-6}}{f'(z)}$

$\frac{b-a}{n} \le \frac{10^{-6}}{z}$

$n \ge \frac{z}{10^{-6}}$

if $n = \frac{1}{10^{-6}} = 10^6$

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 proved 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)

$$I - I_M = \int_a^b f(x)\,dx - \sum_{i=0}^{n-1} h\cdot f(a+\tfrac{1}{2}(i+\tfrac{1}{2})h)$$

$$= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} [f(x) - f(a+\tfrac{1}{2}(i+\tfrac{1}{2})h)]\,dx$$

$$= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} [\cancel{f(a+(i+\tfrac{1}{2})h)} + \frac{f'(a+(i+\tfrac{1}{2})h)}{1!}(x-(a+(i+\tfrac{1}{2})h)) + \frac{f''(z_i)}{2!}(x-(a+(i+\tfrac{1}{2})h))^2 - \cancel{f(a+\tfrac{1}{2}(i+\tfrac{1}{2})h)}]$$

$$= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} \frac{f'(a+(i+\tfrac{1}{2})h)}{1!}(x-(a+(i+\tfrac{1}{2})h)) + \frac{f''(z_i)}{2!}(x-(a+(i+\tfrac{1}{2})h))^2$$

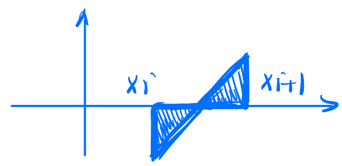
$$① = \sum_{i=0}^{n-1} \frac{f'(a+(i+\tfrac{1}{2})h)}{1!} \underbrace{\int_{x_i}^{x_{i+1}} (x-(a+(i+\tfrac{1}{2})h))\,dx}$$

$$= \tfrac{1}{2}[x-(a+(i+\tfrac{1}{2})h)]^2 \Big|_{x_i}^{x_{i+1}}$$

$$= \tfrac{1}{2}[(\tfrac{1}{2}h)^2 - (\tfrac{1}{2}h)^2]$$

$$= 0$$

$$= 0$$



$$② = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} \underbrace{\frac{f''(z_i)}{2!}}_{\text{constants}} \underbrace{(x-(a+(i+\tfrac{1}{2})h))^2}_{\geq 0 \text{ in } [x_i, x_{i+1}]}\,dx$$

$$= \sum_{i=0}^{n-1} \frac{f''(z_i)}{2!} \underbrace{\int_{x_i}^{x_{i+1}} (x-(a+(i+\tfrac{1}{2})h))^2\,dx}$$

$$\tfrac{1}{3}(x-(a+(i+\tfrac{1}{2})h))^3 \Big|_{x_i}^{x_{i+1}}$$

$$= \tfrac{1}{3}((\tfrac{h}{2})^3 - (-\tfrac{h}{2})^3)$$

$$= \tfrac{1}{3}(\tfrac{2h^3}{8})$$

$$= \sum_{i=0}^{n-1} \frac{f''(z_i')}{2} \cdot \frac{1}{3} \cdot \frac{h^3}{4}$$

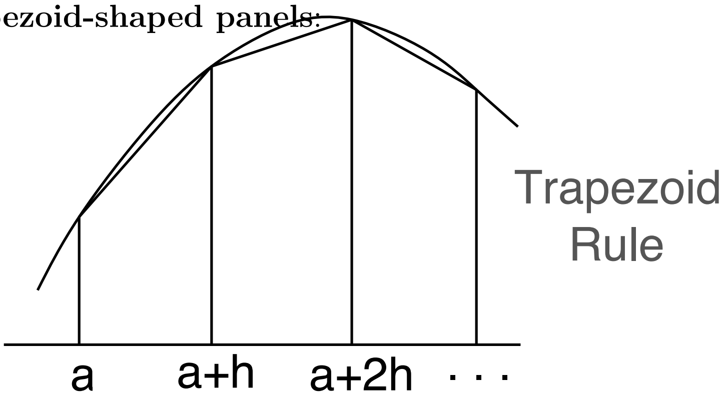
$$= f''(z) \sum_{i=0}^{n-1} \frac{1}{24} h^3$$

$$= f''(z) \frac{h^2}{24} \cdot nh$$

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

Trapezoid Rule

Consider **trapezoid-shaped panels**:



The trapezoid rule:

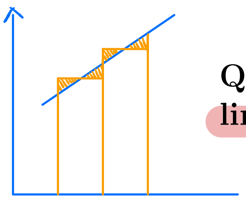
$\sum_{i=0}^{n-1} \frac{1}{2}[f(a+ih)+f(a+(i+1)h)]h$

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

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

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

proof



Q: Show that 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

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

$n=2$

$2 \to 4$

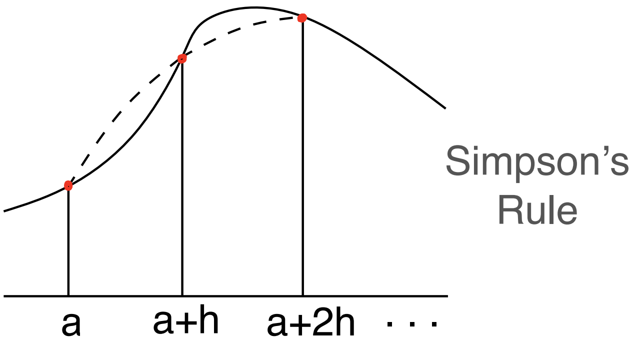
how many new points / improve

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.

We can use the recursive formula to do iterations to compute I. Starting with $n = 1$, we stop iteration when $|I_T(2^n) - I_T(2^{n-1})| \le \delta$, where δ is a tolerance.

Simpson's Rule

There is no need for straight edges:



Each panel is topped by a **parabola**. There is 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

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

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

$$\vdots$$

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

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 $z \in [a, b]$

$$I - I_S = -\frac{1}{180}(b-a)h^4 f^{(4)}(z) = O(h^4).$$ Proof is not testable.

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 vary rapidly on some parts of the interval $[a, b]$, but vary little on other parts. It is not very efficient to use the same 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 $numI = adapt(f, a, b, \delta, \cdots)$
    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| $\leq \delta$, then
        $numI = I_2 +$ the estimated error
    else
        $c = (a + b)/2$
        $numI = adapt(f, a, c, \delta/2, \cdots)$
            $+adapt(f, c, b, \delta/2, \cdots)$
    end

This will guarantee $|I - numI| \lesssim \delta$.
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 $numI = adapt\_simpson(f, a, b, \delta, level, level\_max)$
    $h \leftarrow b - a$
    $c \leftarrow (a + b)/2$
    $I_1 \leftarrow h[f(a) + 4f(c) + f(b)]/6$
    $level \leftarrow level + 1$
    $d \leftarrow (a + c)/2$
    $e \leftarrow (c + b)/2$
    $I_2 \leftarrow h[f(a) + 4f(d) + 2f(c) + 4f(e) + f(b)]/12$
    if $level \geq level\_max$, then
        $numI \leftarrow I_2$
    else
        if $|I_2 - I_1| \leq 15\delta$, then
            $numI \leftarrow I_2 + \frac{1}{15}(I_2 - I_1)$
        else
            $numI \leftarrow adapt\_simpson(f, a, c, \delta/2, level, level\_max)$
                $+ adapt\_simpson(f, c, b, \delta/2, level, level\_max)$
        end
    end

Remark: Like the maximum number of iterations used as a stopping criterion in the Newton method for solving a nonlinear equation, here the maximum number levels $level\_max$ is used to ensure the iteration will terminate.

Don't need to memorize the formulas.

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

condition $$\int_a^b x^k q(x)dx = 0, \qquad k = 0, 1, \ldots, n. \tag{2}$$

Let $x_0, x_1, \ldots, x_n$ be the zeros of $q(x)$. Then for any polynomial $f(x)$ with degree less than or equal to $2n+1$,

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

Lagrange

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

Examples will be given in class to show how to establish some Gaussian quadratic rules such as

$$\int_{-1}^{1} f(x)dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).$$

Interval change. Suppose a Gaussian quadrature rule for $\int_{-1}^{1} f(x)dx$ is

$$I_G[-1, 1] = \sum_{i=0}^{n} A_i f(x_i).$$

We can extend it to compute $\int_a^b f(x)dx$ by an interval transformation. Setting $x = \alpha + \beta t$, where $a = \alpha + \beta(-1)$ and $b = \alpha + \beta$ leads to

$$\alpha = \frac{1}{2}(a + b), \quad \beta = \frac{1}{2}(b - a).$$

Then

$$\int_a^b f(x)dx = \beta \int_{-1}^{1} f(\alpha + \beta t)dt \approx I_G[a, b] \equiv \beta \sum_{i=0}^{n} A_i f(\alpha + \beta x_i).$$