Numerical Integration

Motivation: Many simple functions do not have analytic anti-derivatives,
  e.g. \( e^{-x^2} \), \( \cos(x^2) \), etc.
  However \( \int_a^b e^{-x^2} \, dx \) exists and is finite.

Newton-Cotes Formulas

Strategy: Given \( \int_a^b f(x) \, dx \), replace \( f(x) \) by a polynomial interpolant then integrate the polynomial:

\[
\int_a^b f(x) \, dx \approx \int_a^b P_n(x) \, dx \quad \text{where} \quad P_n(x) \text{ is the } n \text{th degree interpolant of } f(x)
\]
at \( x_0, x_1, \ldots, x_n \).

Recall the \( n \)th degree Lagrange interpolant of \( f(x) \):

\[
P_n(x) = \sum_{i=0}^{n} f(x_i) \prod_{j=0, j \neq i}^{n} \frac{x-x_j}{x_i-x_j}
\]

\[
\int_a^b f(x) \, dx \approx \int_a^b \left( \sum_{i=0}^{n} f(x_i) \prod_{j=0, j \neq i}^{n} \frac{x-x_j}{x_i-x_j} \right) \, dx
\]

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

- This is a definite integral of a polynomial "easy" to do
- Simple summation
- "Thank for loop!"

Approximations derived in this way are called Newton-Cotes formulas —
named after Isaac Newton & Roger Cotes.
Trapezoidal Method

- Assuming $f(x)$ has 2 continuous derivatives on $[x_0, x_1]$.
- Define the Lagrange interpolating polynomial on $(x_0, f(x_0))$ and $(x_1, f(x_1))$

We define the Lagrange interpolating polynomial

$$f(x) = \frac{(x-x_1)}{x_0-x_1} f(x_0) + \frac{(x-x_0)}{x_1-x_0} f(x_1) + \frac{(x-x_0)(x-x_1)}{2!} f''(c)$$

where $c \in (x_0, x_1)$

so that

$$f(x) = P(x) + \text{some error}, \quad (\ast) \quad \text{where } P(x) \text{ is linear.}$$

Integrating both sides of $(\ast)$

$$\int_{x_0}^{x_1} f(x) \, dx = \int_{x_0}^{x_1} \left( \frac{(x-x_1)}{x_0-x_1} f(x_0) + \frac{(x-x_0)}{x_1-x_0} f(x_1) \right) \, dx + \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)}{2!} f''(c) \, dx$$

Computing the first integral yields

$$\int_{x_0}^{x_1} \frac{x-x_1}{x_0-x_1} \, dx + \int_{x_0}^{x_1} \frac{x-x_0}{x_1-x_0} \, dx$$

$$= \frac{x_1-x_0}{2} \left[ f(x_0) + f(x_1) \right]$$

Note: if we let $h = x_1 - x_0$, the integrals above can be evaluated as follows

Let $u = x - x_1$

$$\frac{du}{dx} = 1 \Rightarrow du = dx$$

Changing limits

$x = x_0 \Rightarrow u = x_0 - x_1 = -h$

$x = x_1 \Rightarrow u = x_1 - x_1 = 0$

Next, we quantify the error in the method.
How big is the trapezoidal error?

We have to quantify \[ \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)}{2} f''(\xi) \, dx. \]

**Weighted Mean Value Theorem**

If \( f \) is continuous on \([a, b]\) and \( g(x) \) does not change sign on \([a, b]\), then there exist \( \eta \in [a, b] \) such that

\[
\int_{a}^{b} f(x) g(x) \, dx = f(\eta) \int_{a}^{b} g(x) \, dx.
\]

WLOG, suppose \( g(x) \geq 0 \) on \([a, b]\) (if \( g(x) < 0 \), the proof is similar).

Let \( m \) and \( M \) be the minimum and maximum values of \( g(x) \) for \( x \) on \([a, b]\).

Since \( g(x) \geq 0 \), it follows that

\[
m g(x) \leq f(x) g(x) \leq M g(x), \quad \forall x \in [a, b]
\]

therefore

\[
m \int_{a}^{b} g(x) \, dx \leq \int_{a}^{b} f(x) g(x) \, dx \leq M \int_{a}^{b} g(x) \, dx
\]

If \( \int_{a}^{b} g(x) \, dx = 0 \), any \( \eta \in [a, b] \) will do because \( \int_{a}^{b} f(x) g(x) \, dx = 0 \), otherwise

\[
\int_{a}^{b} g(x) \, dx > 0
\]

so

\[
m \leq \frac{\int_{a}^{b} f(x) g(x) \, dx}{\int_{a}^{b} g(x) \, dx} \leq M
\]

by IVT, there exists \( \eta \in [a, b] \) such that

\[
f(\eta) = \frac{\int_{a}^{b} f(x) g(x) \, dx}{\int_{a}^{b} g(x) \, dx}
\]
\[
\int_{x_0}^{x_1} f(x) \, dx - \int_{x_0}^{x_1} P_i(x) \, dx = \frac{1}{2} \left( \int_{x_0}^{x_1} f''(x) (x-x_0)(x-x_1) \, dx \right) - \frac{1}{12} \left( \int_{x_0}^{x_1} P(x) \, dx \right)^2
\]

Hence,

\[
\int_{x_0}^{x_1} (x-x_0)(x-x_1) \, dx
\]

Let \( u = x - x_0 \) and recall that \( x_1 - x_0 = h \).

Then

\[
\int_{x_0}^{x_1} (x-x_0)(x-x_1) \, dx = \int_{0}^{h} u(u-h) \, du = \left. \frac{u^3}{3} - \frac{u^2 h}{2} \right|_{0}^{h} = \frac{h^3}{3} - \frac{h^3}{2} = -\frac{h^3}{6}
\]

\[
= \frac{1}{2} f''(\eta) \cdot \left( -\frac{h^3}{6} \right)
\]

So we conclude that

\[
\int_{x_0}^{x_1} f(x) \, dx - \int_{x_0}^{x_1} P_i(x) \, dx = -\frac{h^3}{12} f''(\eta)
\]
Simpson's Rule

Replace the degree 1 interpolant with a parabola.

\[ P_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \]

\[
\int_{x_0}^{x_2} f(x) \, dx = \int_{x_0}^{x_1} P_2(x) \, dx + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f^{(4)}(c) \, dx
\]

\[
= f(x_0) \frac{h}{3} + f(x_1) \frac{4h}{3} + f(x_2) \frac{h}{3}, \quad h = x_2 - x_1 = x_1 - x_0
\]

\[
\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f^{(4)}(c) \, dx = -\frac{h^5}{90} f^{(4)}(c)
\]

where \( c \) is on \([x_0, x_2]\), provided \( f^{(4)}(x) \) exists and is continuous.

Alternatively

Method of undetermined coefficients

Derive a formula that is exact for constants, linear and quadratic functions.

The formula has to be exact of the form

\[
\int_{a}^{b} f(x) \, dx = A_1 f(a) + A_2 f\left(\frac{a+b}{2}\right) + A_3 f(b)
\]

Set up a system of 3 equations to ensure that integration is exact for \(1, x, x^2\).

\[
\begin{align*}
 f(a) = 1 & \Rightarrow \int_{a}^{b} 1 \, dx = b-a = A_1 + A_2 + A_3 \quad \text{(i)} \\
 f(x) = x & \Rightarrow \int_{a}^{b} x \, dx = \frac{b^2-a^2}{2} = A_1 a + A_2 \left(\frac{a+b}{2}\right) + A_3 b \quad \text{(ii)} \\
 f(x) = x^2 & \Rightarrow \int_{a}^{b} x^2 \, dx = \frac{b^3-a^3}{3} = A_1 a^2 + A_2 \left(\frac{a+b}{2}\right)^2 + A_3 b^2 \quad \text{(iii)}
\end{align*}
\]

Solving this yields \( A_1 = 2A_0 \frac{b-a}{b} \), \( A_2 = \frac{4}{b} (b-a) \)}
\[ \int_a^b f(x) \, dx = \frac{b-a}{6} \left[ f(a) + 4f\left( \frac{b+a}{2} \right) + f(b) \right] \quad \text{(Simpson's Rule)} \]

The error term is \( \frac{1}{2880} (b-a)^5 f^{(4)}(c) \) for \( c \in [a,b] \).

Notice that the method is exact for polynomials of degree 3 (better than we expected with the set up of (i)-(iii)).

**Degree of Precision**

If a formula has zero error when integrating any polynomial of degree \( \leq r \), and if the error is non-zero for some polynomial of degree \( r+1 \), then we say the formula has degree of precision equal to \( r \).

eg. Simpson's method has degree of precision 3

Trapezoidal has degree of precision 1.

**Example (Method of Undetermined Coefficients)**

Determine \( A_0, A_1 \) and \( A_2 \) so that the formula

\[ \int_{-1}^1 f(x) \, dx = A_0 f\left( \frac{-1}{3} \right) + A_1 f\left( \frac{1}{3} \right) + A_2 f(1) \]

has degree of precision at least 2.

Degree of precision \( \geq 2 \) \( \Rightarrow \) Formula is exact for 1, \( x, x^2 \) so that

\[ f(x) = 1 \]

\[ \int_{-1}^1 1 \, dx = 2 \Rightarrow A_0 + A_1 + A_2 = 2 \quad \ldots \text{(i)} \]

\[ f(x) = x \]

\[ \int_{-1}^1 x \, dx = \left. \frac{x^2}{2} \right|_{-1}^1 = 0 \Rightarrow -\frac{1}{3} A_0 + \frac{1}{3} A_1 + A_2 = 0 \quad \ldots \text{(ii)} \]

\[ f(x) = x^2 \]

\[ \int_{-1}^1 x^2 \, dx = \left. \frac{x^3}{3} \right|_{-1}^1 = \frac{2}{3} \Rightarrow \frac{2}{3} \left( -\frac{1}{3} \right)^2 A_0 + \left( \frac{1}{3} \right)^2 A_1 + A_2 = \frac{2}{3} \quad \ldots \text{(iii)} \]
Solving yields

\[ a_0 = \frac{3}{2}, \quad a_1 = 0, \quad a_2 = \frac{1}{2} \]

Solve using MATLAB

\[
\begin{bmatrix}
1 & 1 & 1 \\
\frac{1}{2} & \frac{1}{2} & 1 \\
\frac{1}{9} & \frac{1}{9} & 1
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2
\end{bmatrix}
= \begin{bmatrix} 2 \\
0 \\
\frac{1}{2}
\end{bmatrix}
\]

The error terms for approximating \[ \int_a^b f(x)dx \]

1. **Trapezoidal**
   \[
   \frac{1}{12} (b-a)^2 f''(c)
   \]

2. **Simpson's Rule**
   \[
   \frac{1}{2880} (b-a)^4 f^{(4)}(c)
   \]

Disadvantage of 1 and 2, if \( (b-a) \) is large, the error is large.
Composite Methods

A. Composite Trapezoidal Method. \( \left( \int_a^b f(x) \, dx \right) \)

1. Split the interval of integration \([a,b] \) into \( n \) subintervals by defining

\[
h = \frac{b-a}{n} \quad \text{and} \quad x_j = a + (j-1)h, \quad 1 \leq j \leq n+1
\]

2. Apply Trapezoidal method on \([x_j, x_{j+1}] \) so that

\[
\int_a^b f(x) \, dx = \sum_{j=1}^{n} \int_{x_j}^{x_{j+1}} f(x) \, dx = \sum_{j=1}^{n} \frac{x_{j+1} - x_j}{2} \left[ f(x_j) + f(x_{j+1}) \right] - \sum_{j=1}^{n} \frac{(x_{j+1} - x_j)^3}{12} f''(c_j)
\]

where \( c_j \in (x_j, x_{j+1}) \).

A closer look at the error term

Assuming \( f \) has 2 continuous derivatives, then the Extreme Value Theorem \( \Rightarrow \) there exists \( c_1, c_2 \in [a,b] \) such that

\[
f''(c_1) = \max f''(x) \quad \text{as } x \in [a,b]
\]

\[
f''(c_2) = \min f''(x) \quad \text{as } x \in [a,b]
\]

This means, for each \( j \)

\[
f''(c_j) \leq f''(c_j') \leq f''(c_2)
\]

Summing over \( n \) intervals

\[
n f''(c_j) \leq \sum_{j=1}^{n} f''(c_j) \leq n f''(c_2) \quad \text{OR} \quad \frac{1}{n} \sum_{j=1}^{n} f''(c_j) \leq f''(c_1) \leq \frac{1}{n} \sum_{j=1}^{n} f''(c_j) \leq f''(c_2)
\]

By the Intermediate Value Theorem, there exists \( c \) in \([a,b]\) such that

\[
f''(c) = \frac{1}{n} \sum_{j=1}^{n} f''(c_j)
\]
\[ n f''(c) = \sum_{j=1}^{n} f''(c_j), \text{ so the error term can be written as} \]

\[
\frac{h^3}{12} \sum_{j=1}^{n} f''(c_j) = \frac{h^3}{12} n f''(c) \text{ then notice that } nh = b - a
\]

so that the error term is \[
\frac{h^2}{12} (b-a) f''(c).
\]

\[
\int_{a}^{b} f(x) dx - \sum_{j=1}^{n} \int_{x_j}^{x_{j+1}} f(x) dx = \frac{h^2}{12} (b-a) f''(c) = O(h^3)
\]

See Demo
Trapezoidal and Simpson's method are examples of closed Newton-Cotes methods in which the endpoints are included in the formula.

**Examples of Open Newton-Cotes Methods**

(i) Midpoint method

\[ \int_{a}^{b} f(x) \, dx \approx (b-a)f\left(\frac{a+b}{2}\right) \]

(ii) \[ \int_{a}^{b} f(x) \, dx = \frac{b-a}{3} \left[ 2f(a+\Delta x) - f(a+2\Delta x) + 2f(a+3\Delta x) \right] \]

where \( \Delta x = \frac{b-a}{3} \) can be obtained by interpolating \( f \) on \( x_0 = a+\Delta x, \quad x_1 = a+2\Delta x \) and integrating the resulting polynomial.
0. Split \([a, b]\) into an even number \(n\) sub-intervals \(n = 2m\), \(h = \frac{b - a}{2m}\)

\[
\int_a^b f(x) \, dx = \sum_{j=1}^{m} \int_{x_{2j-1}}^{x_{2j+1}} f(x) \, dx = \sum_{j=1}^{m} \frac{x_{2j+1} - x_{2j-1}}{6} \left[ f(x_{2j-1}) + 4f(x_{2j}) + f(x_{2j+1}) \right] - \sum_{j=1}^{m} \frac{(x_{2j+1} - x_{2j-1})^5}{2880} f^{(4)}(c_j)
\]

\[
= \frac{h}{3} \left[ f(x_1) + 4 \sum_{j=1}^{m} f(x_{2j}) + 2 \sum_{j=1}^{m-1} f(x_{2j+1}) + f(x_{2m+1}) \right] - \sum_{j=1}^{m} \frac{(2h)^5}{2880} f^{(4)}(c_j)
\]

The error term can be rewritten in the same way as the Trapezoidal method as

\[
\sum_{j=1}^{m} \frac{(2h)^5}{2880} f^{(4)}(c_j) = \frac{h^5}{90} \sum_{j=1}^{m} f^{(4)}(c_j)
\]

\[
= \frac{(b-a) h^5}{90} n f^{(4)}(c) \quad \text{(and recall that} \quad h n = \frac{b-a}{2})
\]

\[
= \frac{(b-a) h^4}{180} f^{(4)}(c).
\]
Choosing \( n \) (\# of sub-intervals) for Composite Methods

**Objective**

Compute \( \int_0^1 e^{-x^4} \, dx \) so that the error is no more than \( 1.0 \times 10^{-5} \) using

(a) **Trapezoidal Rule**

The error is

\[
\text{Error} = \frac{(b-a)}{12} h^2 f''(c), \text{ in this case } h \text{ becomes}
\]

\[
- \frac{(1-a)^2}{12} \left( \frac{1}{h^2} \right) f''(c) \quad \text{for some } c \in [0,1]. \quad (h = \frac{1}{n})
\]

We need to choose \( n \) so that

\[
\frac{1}{12n^2} \max_{0 \leq x \leq 1} |f''(x)| < 10^{-5}
\]

For \( f(x) = e^{-x^4} \), it can be shown that \( \max_{0 \leq x \leq 1} |f''(x)| < 3.5 \) so

\[
\frac{3.5}{12n^2} < 10^{-5} \implies n > \sqrt{\frac{3.5}{12 \times 10^{-5}}} \quad n > 170.78
\]

So choose \( n = 171 \).

(b) **Simpson's Method**

\[
\left(1 - \frac{1}{4}\right) \max_{0 \leq x \leq 1} |f^{(4)}(x)| \quad < \quad 1.0 \times 10^{-5}
\]

\[
\frac{180n^4}{180n^4} \max_{0 \leq x \leq 1} |f^{(4)}(x)| < 95
\]

\[
\frac{95}{180n^4} < 1.0 \times 10^{-5} \implies n \approx 16
\]
Gaussian Integration

So far we have obtained integration methods via "interpolate then integrate."

**Alternative Question**

Obtain rules by ensuring that we can integrate the largest possible degree.

**Motivation**

Let \( f(x) \) be continuous on \([a,b]\)

\[
\max_{a \leq x \leq b} |f(x) - P_n(x)| \to 0 \quad \text{as } n \text{ increases},
\]

where \( P_n(x) \) approximates \( f(x) \).

**Strategy**

Fix the interval of integration to \( \int_a^b f(x) \, dx \) and derive a formula of the form

\[
\int_{-1}^{1} f(x) \, dx = \sum_{j=1}^{n} w_j f(x_j)
\]

where \( \{x_1, x_2, \ldots, x_n\} \) are nodes on \([-1,1]\) and

\( \{w_1, w_2, \ldots, w_n\} \) are weights chosen to maximize the degree of precision of the formula.

\( n=1 \)

\[
\int_{-1}^{1} f(x) \, dx = w_1 f(x_1)
\]

We have 2 degrees of freedom \((x_1, w_1)\) so we can ensure exact integration for \( f(x) = 1 \)

\[
f(x) = 1 \quad \Rightarrow \quad \int_{-1}^{1} dx = 2 \quad \Rightarrow w_1 = 2
\]

\[
f(x) = x \quad \Rightarrow \quad \int_{-1}^{1} x \, dx = x^2 \bigg|_{-1}^{1} = 0 \quad \Rightarrow \quad 2 \cdot x_1 = 0 \quad \Rightarrow \quad x_1 = 0
\]

\[
\int_{-1}^{1} f(x) \, dx = 2f(0) \quad \text{[Midpoint Rule]}
\]
In general given $2n$ parameters $\{x_1, x_2, \ldots, x_n, w_1, w_2, \ldots, w_n\}$ we can force the formulas to be exact for polynomials of degree $2n-1$, using a system of $2n$ equations.

The system is hard to solve but published tables of solution values exist. (See slides).

\[ \int_{a}^{b} f(x) \, dx = \sum_{i=1}^{n} w_i f(x_i) \]

What if the integral is defined on $[a, b]$?

Perform a change of variables.

Let $x = \frac{(b + a) + t(b - a)}{2}$, $-1 \leq t \leq 1$

\[ \frac{dx}{dt} = \frac{b - a}{2} \]

\[ \int_{a}^{b} f(x) \, dx = \int_{-1}^{1} f \left( \frac{(b + a) + t(b - a)}{2} \right) \left( \frac{b - a}{2} \right) dt \]

\[ = \frac{b - a}{2} \int_{-1}^{1} f \left( \frac{(b + a) + t(b - a)}{2} \right) dt = \sum_{i=1}^{n} w_i \frac{(b - a)}{2} f \left( \frac{(b + a) + x_i(b - a)}{2} \right) \]

In general,

\[ \int_{a}^{b} f(x) \, dx = \sum_{i=1}^{n} \tilde{w}_i f(\tilde{x}_i) \]

\[ \tilde{x}_i = \frac{b + a + x_i(b - a)}{2} \]

\[ \tilde{w}_i = w_i \frac{b - a}{2} \]

\[ x = \frac{(b + a) + t(b - a)}{2} \]

Map:

Integral to "reference interval!"
for \( f(x) = x^2 \), check
\[
\int_{-1}^{1} x^2 \, dx = \left. \frac{x^3}{3} \right|_{-1}^{1} = \frac{2}{3}.
\]
the approximation is 0 so the degree of precision is 1.

\( n=2 \)
\[
\int_{-1}^{1} f(x) \, dx = w_1 f(x_1) + w_2 f(x_2)
\]
We have 4 unknowns so we can impose 4 conditions:

The rule is exact on 1, \( x \), \( x^2 \), \( x^3 \) yielding
\[
\begin{align*}
2 &= w_1 + w_2, \quad \text{(i)} \\
0 &= w_1 x_1 + w_2 x_2, \quad \text{(ii)} \\
\frac{2}{3} &= w_1 x_1^2 + w_2 x_2^2, \quad \text{(iii)} \\
0 &= w_1 x_1^3 + w_2 x_2^3, \quad \text{(iv)}
\end{align*}
\]
The solution is
\[
\begin{align*}
w_1 &= w_2 = 1, \\
x_2 &= -\frac{\sqrt{3}}{3}, \\
x_3 &= \frac{\sqrt{3}}{3},
\end{align*}
\]
\[
\int_{-1}^{1} f(x) \, dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)
\]

degree of precision

Check \( n = 4 \), \( x^4 \).

Exact
\[
\int_{-1}^{1} x^4 \, dx = \left. \frac{x^5}{5} \right|_{-1}^{1} = \frac{2}{5}
\]

Approx
\[
\begin{align*}
f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) &= \left(-\frac{1}{\sqrt{3}}\right)^4 + \left(\frac{1}{\sqrt{3}}\right)^4 \\
&= \frac{2}{9} \neq \frac{2}{5}
\end{align*}
\]
So the degree of precision is 3.
**Periodic Integrals**

A function $f$ is periodic with period $T$ if $f(x) = f(x+T)$, $-\infty < x < \infty$

**Example**: $f(x) = e^{\cos(2\pi x)}$

**Fact**

If $f(x)$ is periodic with period $T$, then the derivatives are also periodic with period $T$.

**Trapezoidal Method**

\[ -\frac{1}{12} h^3 \sum_{i=1}^{n} f''(c_i) = -\frac{h^2}{12} \left[ h f''(c_1) + h f''(c_2) + \cdots + h f''(c_n) \right] \]

Note that $\sum_{i=1}^{n} f''(c_i)h \approx$ is the Riemann sum of $\int_a^b f''(x)dx = f'(b) - f'(a)$

This means that as $h \to 0 \ (n \to \infty)$, the Trapezoidal error is

\[ -\frac{h^2}{12} \left[ f'(b) - f'(a) \right] \to 0 \text{ at a rate faster than } O(h) \]

If $f$ is periodic $f''(b) = f''(a)$ so this term $\to 0$

This term also $\to 0$

**Simpson's Method**

\[ \text{Error} \approx -\frac{h^4}{180} \left[ f'''(b) - f'''(a) \right] \to 0 \text{ at a rate faster than } O(h^4) \]

For periodic functions