Lecture on
Numerical Integration

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[Approx. chap. 5.2 in Sauer]
Numerical integration (Quadrature)

When is numerical integration needed? Examples:

\[
\int \frac{dx}{\log x} \quad \int e^{-x^2} \, dx \quad \int \sqrt{1 + \cos^2 x} \, dx
\]

No primitive function in terms of elementary functions.

**Numerical integration:** Discretization

\[
\int_a^b f(x) \, dx \quad \rightarrow \quad \sum_i f(x_i) \Delta x
\]
Numerical integration…

\[ \int_{a}^{b} f(x) \, dx \quad \rightarrow \quad \sum_{i} f(x_i) \Delta x \]

Compare lower and upper Riemann sums.
Basic idea of quadrature methods

Integrals of polynomials can be computed exactly.

Approximate \( f(x) \) by a polynomial \( P(x) \). Then

\[
\int_{a}^{b} f(x) \, dx \approx \int_{a}^{b} P(x) \, dx.
\]

Computable integral approximates non-computable one.

**Composite quadrature:** High accuracy requires high degree polynomials. Use low degree on many subintervals instead.

\[
\int_{a}^{b} f(x) \, dx = \sum_{j} \int_{x_{j-1}}^{x_{j}} f(x) \, dx \approx \sum_{j} \int_{x_{j-1}}^{x_{j}} P_j(x) \, dx
\]

where \( a = x_0 < x_1 < \ldots < x_N = b \).
Example: Lagrange interpolation

Interpolation polynomial

\[ P(x) = \sum_{i=0}^{n} f(x_i)\varphi_i(x) \quad \Rightarrow \]

\[ \int_{a}^{b} P(x) \, dx = \int_{a}^{b} \sum_{i=0}^{n} f(x_i)\varphi_i(x) \, dx \]

\[ = \sum_{i=0}^{n} f(x_i) \int_{a}^{b} \varphi_i(x) \, dx = \sum_{i=0}^{n} w_i f(x_i) \]

All quadrature methods replace the integral by a weighted sum of \( f \)–values.
Newton–Cotes quadrature

Interpolate the integrand by polynomial of degree $n$,

$$\int_a^b f(x) \, dx = \int_a^b P(x) \, dx + \text{Error}$$

Closed Newton–Cotes methods:
Include interval endpoints among interpolation points.

- $n = 1$: Trapezoidal rule
- $n = 2$: Simpson’s rule

Open Newton–Cotes methods:
Exclude interval endpoints from interpolation points.

- $n = 0$: Midpoint rule
The Trapezoidal rule (closed with $n = 1$)

Use Lagrange polynomials

$$\varphi_0(x) = \frac{x - b}{a - b} \quad \text{and} \quad \varphi_1(x) = \frac{x - a}{b - a}.$$ 

This gives the weights

$$w_0 = \int_a^b \varphi_0(x) \, dx = \frac{1}{2}(b - a) \quad \text{and} \quad w_1 = \frac{1}{2}(b - a).$$

Hence, $P(x) = f(a)\varphi_0(x) + f(b)\varphi_1(x)$ and

$$\int_a^b f(x) \, dx \approx \int_a^b P(x) \, dx = \frac{1}{2}(b - a)(f(a) + f(b)).$$
Error for the Trapezoid rule

Let $\Delta x = b - a$, then

$$
\int_a^b f(x) \, dx = \frac{1}{2} \Delta x (f(a) + f(b)) + E
$$

The interpolation error is

$$
e(x) = f(x) - P(x) = \frac{1}{2} f''(\xi) (x - a)(x - b)
$$

and the quadrature error $E$ is then

$$
E = \int_a^b e(x) \, dx = \int_a^b \frac{1}{2} f''(\xi) (x - a)(x - b) \, dx
$$

$$
= \frac{1}{2} f''(c) \int_a^b (x - a)(x - b) \, dx
$$

$$
= -\frac{1}{12} \Delta x^3 f''(c).
$$
The Midpoint rule (open with $n = 0$)

Interpolate with a constant at the midpoint $(a + b)/2$.

Let $x_0 = (a + b)/2$ and $P(x) = f(x_0) \cdot 1$.

This gives the approximation

$$\int_a^b f(x) \, dx \approx \int_a^b P(x) \, dx = (b - a)f\left(\frac{1}{2}(a + b)\right).$$
Error for the Midpoint rule

Set $\Delta x = b - a$ and $m = (a + b)/2$, then

$$\int_a^b f(x) \, dx = \Delta x \, f(m) + E$$

Taylor expanding $f(x)$ around $m$ gives

$$\int_a^b f(x) \, dx = \int_a^b f(m) + f'(m)(x - m) + \frac{1}{2}f''(\xi(x))(x - m)^2 \, dx$$

$$= \Delta x \, f(m) + 0 + \frac{1}{2}f''(c) \int_a^b (x - m)^2 \, dx$$

$$= \Delta x \, f(m) + \frac{1}{24}\Delta x^3 f''(c).$$

Hence, $E = 1/24 \Delta x^3 f''(c)$. 
Simpson’s rule (closed with $n = 2$)

Quadratic interpolation at

$$a, \quad (a + b)/2 \quad \text{and} \quad b$$

yields the weights

$$w_0 = (b - a)/6, \quad w_1 = 4(b - a)/6$$
and

$$w_2 = (b - a)/6.$$

Let $\Delta x = b - a$, then one obtains

$$\int_a^b f(x) \, dx = \frac{1}{6} \Delta x \left( f(a) + 4f\left(\frac{1}{2}(a + b)\right) + f(b) \right)$$

$$- \frac{1}{2880} \Delta x^5 f^{(4)}(c)$$
Composite quadrature

Divide the interval \([a, b]\) into \(N\) (equally sized) subintervals with

\[
a = x_0 < x_1 < \ldots < x_N = b
\]

and \(\Delta x = (b - a)/N\).

One then has that

\[
\int_a^b f(x) \, dx = \sum_{j=1}^{N} \int_{x_{j-1}}^{x_j} P_j(x) \, dx + E_j.
\]

Total error:

\[
E_j = \mathcal{O}(\Delta x^{k+1}) \quad \Rightarrow \quad \sum_j E_j = \mathcal{O}(N\Delta x^{k+1}) = \mathcal{O}(\Delta x^k).
\]
Composite quadrature...

Trapezoid rule

\[ \int_{a}^{b} f(x) \, dx = \sum_{j=1}^{N} \frac{1}{2} \left( f(x_{j-1}) + f(x_j) \right) \Delta x + E_j \]

\[ = \Delta x \left( \frac{1}{2} f_0 + f_1 + \cdots + f_{N-1} + \frac{1}{2} f_N \right) + O(\Delta x^2) \]

Midpoint rule

\[ \int_{a}^{b} f(x) \, dx = \Delta x \left( f_{1/2} + f_{3/2} + \cdots + f_{N-1/2} \right) + O(\Delta x^2) \]

Simpson’s rule

\[ \int_{a}^{b} f(x) \, dx = \frac{1}{6} \Delta x \left( f_0 + 4f_{1/2} + 2f_1 + 4f_{3/2} + \cdots + 4f_{N-1/2} + f_N \right) + O(\Delta x^4) \]