Numerical integration.

Exact integration is useful, for example in differential equation, but we need to be able to find anti-derivative.

This is not always possible.

Consider $\int e^{-x^2} dx$.

How do we solve this problem?

① Taylor series (about $x = 0$)

$$e^{-x^2} = 1 - x^2 + \frac{x^4}{2} - \frac{x^6}{3} + \cdots$$

② Approximate the area under the curve.

Riemann sum.

One way to approximate the integral is Riemann sums.

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i^*)\,\Delta x$$

$x_i^* \in [x_{i-1}, x_i]$.

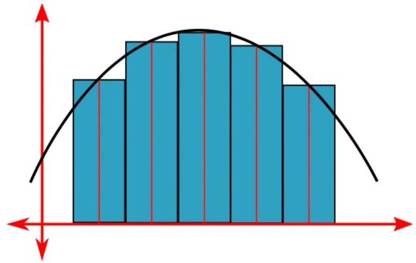
- Left endpoint, $x_i^* = x_{i-1}$
- Right endpoint, $x_i^* = x_i$
- Mid-point, $x_i^* = (x_{i-1} + x_i)/2$.

Thm: (Midpoint rule)

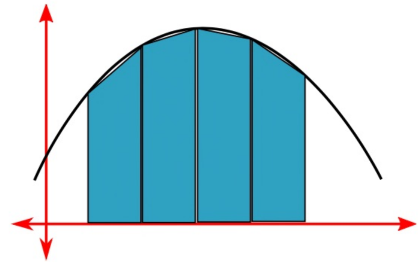
$$\int_a^b f(x)\,dx \approx M_n = \sum_{i=1}^{n} f(\bar{x}_i)\,\Delta x$$

$$\Delta x = \frac{b-a}{n}, \quad x_i = a + i\,\Delta x, \quad \bar{x}_i = (x_{i-1} + x_i)/2.$$

Trapezoid approximation



midpoint

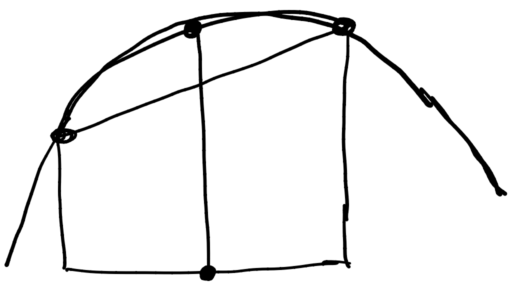


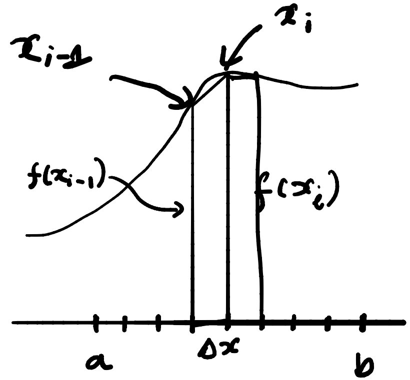
trapezoid

- Trapezoid rule approximates the area under curve using little trapezoid.
- Approximate $f(x)$ on $[x_{i-1}, x_i]$ using a line.

The function $f(x)$ on $[a,b]$ is approximated as a sequence of lines.

Trapezoid rule.





$$\text{Area} = \frac{f(x_i) + f(x_{i-1})}{2} \cdot \Delta x.$$

$$\Delta x = \frac{b-a}{n}$$

Theorem (Trapezoid rule)

$$\int_a^b f(x)\,dx \approx T_n$$

$$= \sum_{i=1}^{n} \frac{\left(f(x_{i-1}) + f(x_i)\right)}{2} \cdot \Delta x$$

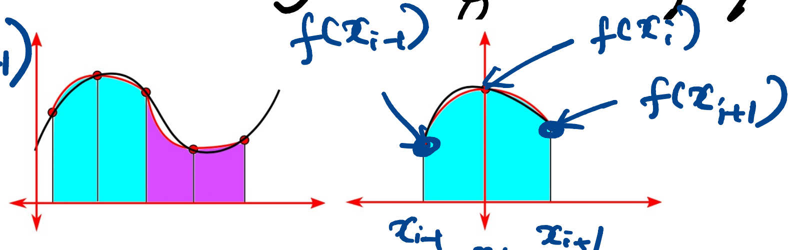
$$= \frac{\Delta x}{2}\left(f(x_0) + 2f(x_1) + 2f(x_2) + \dots + 2f(x_{n-1}) + f(x_n)\right)$$

$$\Delta x = \frac{b-a}{n}, \quad x_i = a + i\,\Delta x.$$

Simpson's rule.

Approximate the curve by a sequence of parabola.

$\frac{\Delta x}{3}(y_{i-1} + 4y_i + y_{i+1})$



The general equation of parabola is $y(x) = Ax^2 + Bx + C$.

- Divide $[a, b]$ into n segments. $\Delta x = (b-a)/n$.
- Approximate $f(x)$ on $[x_{i-1}, x_{i+1}]$ using a parabola.
  i.e find the area of parabola that goes through points.
  $(x_{i-1}, f(x_{i-1}))$, $(x_i, f(x_i))$, $(x_{i+1}, f(x_{i+1}))$
- Add up the area of each parabola

Simpson's rule.

Area of parabola that can be defined by

$$(x_{i-1}, f(x_{i-1})), \quad (x_i, f(x_i)), \quad (x_{i+1}, f(x_{i+1}))$$

is equal to area of parabola defined by.

$$(-\Delta x, f(x_{i-1})), (0, f(x_i)), (\Delta x, f(x_{i+1}))$$

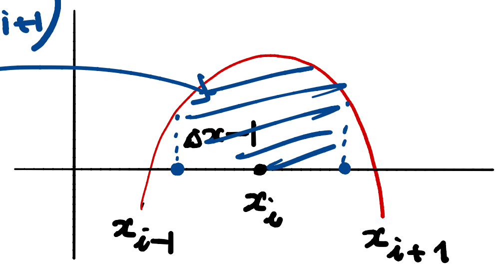
or,

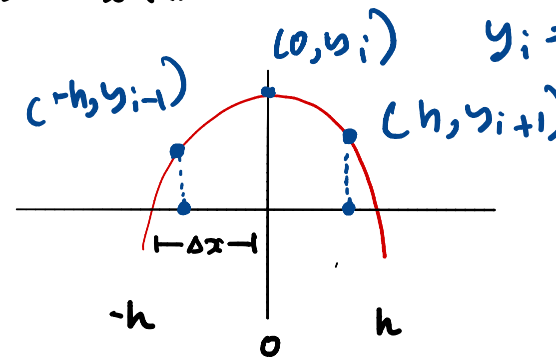
$$(-h, y_{i-1}), (0, y_i) \ (h, y_{i+1}).$$

. let $h = \Delta x$

$y_i = f(x_i)$.

$$\frac{\Delta x}{3}\left(y_{i-1} + 4y_i + y_{i+1}\right)$$





Remark: number of segments $[x_{i-1}, x_i]$ is even.

Area of a little parabola.

Area of parabola given by $\int_{-h}^{h} Ax^2 + Bx + C \, dx$ is.

$$\text{Area} = \left.\frac{Ax^3}{3} + \frac{Bx^2}{2} + Cx\right]_{-h}^{h} = 2Ah^3/3 + 2Ch = \frac{h}{3}(2Ah^2 + 6C).$$

And, $(-h, y_{i-1})$ satisfies $Ah^2 - Bh + C = y_{i-1}$ —— (I)

$(0, y_i)$ satisfies $A \cdot 0^2 - B \cdot 0 + C = y_i$ —— (II)

(h, y_{i+1}) satisfies $Ah^2 + Bh + C = y_{i+1}$ —— (III)

So, from (II) $C = y_i$, combine (I) & (III) to get

$$A = (y_{i-1} + y_{i+1} - 2y_i)/2h^2$$

So. $\text{Area} = \frac{h}{3}(y_{i-1} + y_{i+1} - 2y_i + 6y_i) = \frac{h}{3}(y_{i-1} + 4y_i + y_{i+1})$

Simpson's rule.

To approximate $\int_a^b f(x)\,dx$, add areas of little parabolas.

$$\text{Area} = \frac{h}{3}\left(y_{i-1} + 4y_i + y_{i+1}\right), \qquad h = \Delta x, \quad y_i = f(x_i).$$

Theorem (Simpson's rule).

$f(x_2) + f(x_2)$

$$\int_a^b f(x)\,dx \approx S_n$$

$$= \frac{\Delta x}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big]$$

where $\Delta x = \frac{b-a}{n}$. and n is even.

Error in approximation.

$\text{Error}(n) \leq f(\text{gradient}, n)$

The approximation error is the difference between our approximation and the value of integral. i.e.

depends on n $\rightarrow$ $$\text{Error}(n) = \left| \int_a^b f(x)\,dx - M_n \right|$$ (if using mid point rule)

- As $n \to \infty$, the error goes to zero. (think Riemann sum). How quickly does error go to zero?
- The decay rate of error depends on how "curvy" is the function which is characterized by gradient.
- Error depends on higher order derivatives if approximation uses higher order polynomial

Midpoint, Trapezoid – 2^{nd} order derivative.

Simpson rule – 4^{th} order derivative.

Error bound.

Theorem. (CLP - 1.11.13).

Suppose that $|f''(x)| < K$ on $a \le x \le b$.
Suppose that $|f^{(4)}(x)| < L$ on $a \le x \le b$

If $E_M(n)$, $E_T(n)$ and $E_S(n)$ are the errors of the midpoint rule, trapezoid rule and simpson's rule respectively then.

- $E_T(n) \le \dfrac{K(b-a)^3}{12n^2}$
- $E_M(n) \le \dfrac{K(b-a)^3}{24n^2}$
- $E_S(n) \le \dfrac{L(b-a)^5}{180n^4}$

$n^4 > n^2$

Midpoint is slightly better than trapizoid but Simpson is best

Example

Approximate $\int_1^2 \frac{1}{x}\,dx$ using trapezoid rule and $n=5$.

Sol^n: $T_n = \frac{\Delta x}{2}\left(f(x_0) + 2f(x_1) + 2f(x_2) + \dots + 2f(x_{n-1}) + f(x_n)\right)$

$a = 1, \quad b = 2, \quad \Delta x = 1/5 = 0.2.$

So, $T_n = 0.1\left(f(1) + 2f(1.2) + 2f(1.4) + 2f(1.8) + f(2)\right)$

$= 0.6956\ldots$

$$E_T(n) \leq \frac{k(b-a)^3}{12n^2}$$

Error in approximation.

Consider some question: $\int_1^2 \frac{1}{x}\,dx$. using trapezoid rule & $n=5$.

Exact answer: $\int_1^2 \frac{1}{x}\,dx = \ln|x|\Big|_1^2 = \ln|2| - \ln|1| = \ln 2$

$= 0.6931\ldots$

Lets use error bound theorem to provide a bound on approximation and compare to exact error.

so, $f'(x) = 1/x^2$, $f''(x) = -2/x^3$.

note that $|f''(x)| \leq 2$ on $1 \leq x \leq 2$

so, $E_T(5) \leq \frac{k(b-a)^3}{12n^2} = \frac{2}{12\cdot 5^2} = \frac{1}{150} \approx 0.00666\ldots$

Exact error:

$E_T(5) = \left| \int_a^b f(x)\,dx - T_5 \right| = \left| 0.6931 - 0.6956 \right| = 0.0025.$

Example.

Consider some integral $\int_1^2 \frac{1}{x}\,dx$ using trapezoid

How big do we need n to be in order for the error to less that 10^{-6}?

so, we need $E_T(n) \leq 10^{-6}$

so, we need $10^{-6} \geq \frac{K(b-a)^3}{12n^2} = \frac{2}{12n^2}$

$$\iff n^2 \geq \frac{2}{12\cdot 10^{-6}}$$

$$\iff n \geq \sqrt{\frac{10^6}{36}} \approx 408.25.$$

$$E_T(n) \leq \frac{K(b-a)^3}{12n^2} \leq 10^{-6}$$

Example.

Consider some integral $\int_1^2 \frac{1}{x}\,dx$ using Simpson's rule

How big do we need n to be in order for the error to less that 10^{-6}?

Sol^n: The 4^{th} derivative is $24/x^5$. so,

$$|f^{(4)}(x)| \leq 24 \quad \text{on} \quad 1 \leq x \leq 2$$

we need

$$10^{-6} \geq \frac{L(b-a)^5}{180\, n^4}$$

$$\iff \quad n^4 \geq \frac{24}{180\, 10^{-6}}$$

$$\iff \quad n \geq \left(\frac{2}{15} 10^{-6}\right)^{1/4} \approx 19.1$$