Numerical derivatives

- Backward difference quotient
- Forward ——— " ———

} 1^{st} order $\mathcal{O}(h)$

- Central ——— " ——— 2^{nd} order $\mathcal{O}(h^2)$

Taylor series expansion used for error analysis

Richardson extrapolation:

Use an approximation φ for h and $\frac{h}{2}$.
Look at the error (coming from Taylor series expansion). Combine the estimates for $\varphi(h)$ and $\varphi(\frac{h}{2})$ so that the low order error terms cancel out:

For central differencing:

$$\frac{4\varphi(\frac{h}{2}) - \varphi(h)}{3}$$

yields an approximation of $\mathcal{O}(h^4)$.

5.4 Integration:

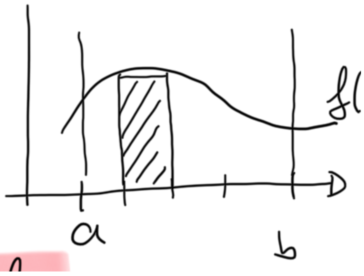
Numerical integration is needed when anti-derivatives can not be easily found.

Recall from Calculus II:

Assume $f \geq 0$ integrable, $f: [a,b] \longrightarrow \mathbb{R}$

Riemann sums:

(1) Partition P of $[a,b]$.
Introduce nodes
$a = x_0 < x_1 < \dots < x_n = b$



and so introduce sub-intervals $[x_i, x_{i+1}]$ for $i = 0, \dots, n-1$

(2) Approximate the area under the curve by summing up areas of rectangles

$$\sum_{i=0}^{n-1} \underbrace{(x_{i+1} - x_i)}_{\text{width}} \underbrace{f(x_i^*)}_{\text{height}} \qquad \underline{\text{Riemann sum}}$$

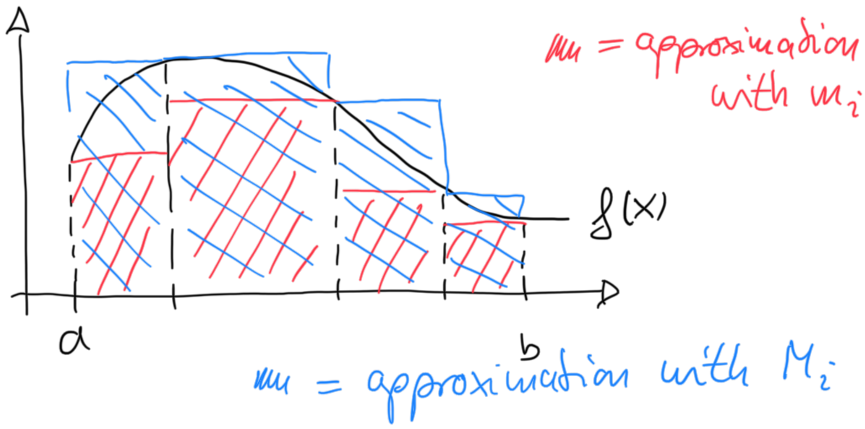
where $x_i^* \in [x_i, x_{i+1}]$

(3) If f is continuous then x_i^* may be chose arbitrarily in $[x_i, x_{i+1}]$. Two choices are interesting:

choose x_i^* such that $f(x_i^*) = \min\{f(x) \mid x_i \le x \le x_{i+1}\} =: m_i$

<u>OR</u>

choose x_i^* such that $f(x_i^*) = \max\{f(x) \mid x_i \le x \le x_{i+1}\} =: M_i$



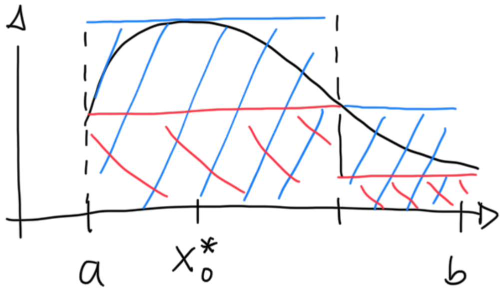
(4) Then,

$$L(f; P) = \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, m_i \qquad \underline{\text{lower sum}}$$

$$U(f; P) = \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, M_i \qquad \underline{\text{upper sum}}$$

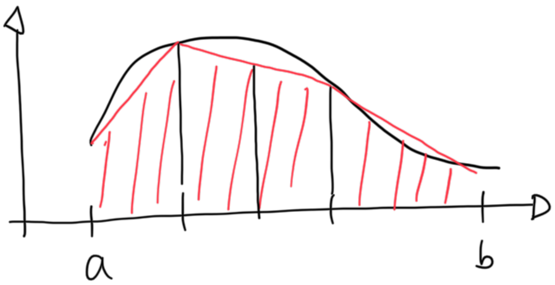
Obviously:

$$L(f;P) \leq \int_a^b f(x)\,dx \leq U(f;P)$$



<u>Trapezoidal rule</u> (like averaging between lower and upper sum)

<u>Idea</u>: Use trapezoids to approximate the area under the graph.



Again, let P be a partition with x_i, $i = 0, \dots, n$, $x_0 = a$, $x_n = b$. In each subinterval the integral is approximated by:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \underbrace{(x_{i+1} - x_i)}_{\text{width of base}} \; \underbrace{\frac{f(x_{i+1}) + f(x_i)}{2}}_{\text{average height of trapezoid}}$$

Summing over all sub-intervals:

$$\boxed{T(f;P) = \frac{1}{2}\sum_{i=0}^{n-1}(x_{i+1}-x_i)\left[f(x_{i+1})+f(x_i)\right]}$$

If the partition is equidistant, i.e. $x_{i+1}-x_i = h$ we get

$$\boxed{T(f;P) = \frac{h}{2}\sum_{i=0}^{n-1}\left[f(x_{i+1})+f(x_i)\right]}$$

Theorem 44: Let $f \in C^2([a,b])$ and P an equidistant partition of $[a,b]$. Then, the error of the trapezoidal rule is

$$\left|\int_a^b f(x)\,dx - T(f;P)\right| = \frac{1}{12}\left|(b-a)h^2 f''(\xi)\right|$$

where $\xi \in (a,b)$, $h = x_{i+1}-x_i$.

It is particularly interesting to use the trapezoidal rule for $n = 2^m$, i.e. $2, 4, 8, 16, \dots$ subintervals. For these partitions it is possible to derive a recursive trapezoidal rule:

$$\boxed{T_m(f;P) = \frac{1}{2}T_{m-1}(f;P) + \dots}$$

Can be used for iteratively refining the result of the approximation.

Romberg algorithm (Romberg 1909 - 2003)

Idea: Use trapezoidal rule and Richardson extrapolation.

First: Use the trapezoidal rule for a sequence of partitions $n = 2^0, 2^1, 2^2, \ldots, 2^m$ for some $m \in \mathbb{N}$.

This yields approximations of the integral

$$R_i^0 := T_i(f; P)$$

trapezoidal rule for 2^i sub interva[ls] i.e. $h = \frac{b-a}{2^i}$

These numbers yield a first column in the Romberg array

$$\begin{array}{ll}
R_0^0 & \\
R_1^0 & R_1^1 \\
R_2^0 & R_2^1 \\
\vdots & \vdots \\
R_m^0 & R_m^1
\end{array}$$

obtained by Richardson extrapolation

Second: Write down the error in Taylor series expansion:

trapezoidal rule for 2^{i-1} sub intervals

$$\int_a^b f(x)\,dx = R_{i-1}^0 + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots \quad (\mathrm{I})$$

note that only even powers appear!

trapezoidal rule for 2^i sub intervals

$$\int_a^b f(x)\,dx = R_i^0 + a_2\left(\frac{h}{2}\right)^2 + a_4\left(\frac{h}{2}\right)^4 + a_6\left(\frac{h}{2}\right)^6 + \quad (\mathrm{II})$$

$$= R_i^0 + \frac{a_2}{4} h^2 + \frac{a_4}{16} h^4 + \frac{a_6}{64} h^6 + \ldots$$

Take $\mathrm{I} - 4 \times \mathrm{II}$:

$$-3\int_a^b f(x)\,dx = \left(R_{i-1}^0 - 4R_i^0\right) + \frac{3}{4} a_4 h^4 + \frac{15}{16} a_6 h^6 + \ldots$$

$$\Leftrightarrow \int_a^b \ldots \quad R_{i-1}^0 - 4R_i^0 \quad a_4 \; h^4 \quad 5 \ldots h^6 +$$

$$\Longleftrightarrow \int_a f(x)\,dx = \underbrace{\frac{\cdots}{-3}}_{R_i^1} - \underbrace{\frac{\cdot}{4}h^{\cdot} - \frac{\cdot}{16}\cdot h^6 \cdots}_{\text{error } \mathcal{O}(h^4)}$$

so $\boxed{R_i^1 = \frac{4}{3}R_i^0 - \frac{1}{3}R_{i-1}^0}$ is a better approximation

Repeat this process to yield a second column in the Romberg array

$$\begin{array}{ccccc}
R_0^0 & & & & \\
R_1^0 & R_1^1 & & & \\
\vdots & R_2^1 & R_2^2 & & \\
\vdots & \vdots & R_3^2 & \ddots & \\
R_m^0 & R_m^1 & R_m^2 & \cdots & R_m^m
\end{array}$$

further columns produced by Richardson extrapolation.

<u>Example:</u>

a   b

$R_0^0 = T_0(f;P)$ i.e. $2^0 = 1$ subinterval
$h_0 = (b-a)$

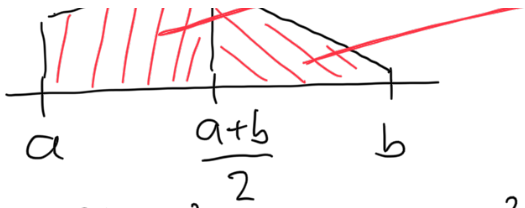
$R_1^0 = T_1(f;P)$ i.e. $2^1 = 2$ subintervals
$h_1 = \frac{b-a}{2} = \frac{h_0}{2}$

$R_2^0 = T_2(f;P)$ i.e. $2^2 = 4$ subintervals
$h_2 = \frac{b-a}{4} = \frac{h_1}{2}$

in more detail:

$R_0^0 = T_0(f;P) = (b-a)\frac{f(b)+f(a)}{2}$ one trapezoid

$$R_0^1 = T_1(f;P) = \frac{b-a}{2}\left[\underbrace{\frac{f\left(\frac{b+a}{2}\right)+f(a)}{2}} + \underbrace{\frac{f(b)+f\left(\frac{b+a}{2}\right)}{2}}\right.$$



<u>Example 45:</u> If $R_3^2 = 1$ and $R_4^2 = 8$

In general we need the following combinati

$$\boxed{R_i^k = R_i^{k-1} + \frac{1}{4^k - 1}\left(R_i^{k-1} - R_{i-1}^{k-1}\right)}$$

<u>Here:</u>

$$R_4^3 = R_4^2 + \frac{1}{4^3 - 1}\left(R_4^2 - R_3^2\right)$$

$$= 8 + \frac{1}{63}(8 - 1)$$

$$= \frac{73}{9} \approx 8.\overline{1}$$

In this formula, the value resulting from more intervals has a greater influence.