

109titration

B-MAT-200

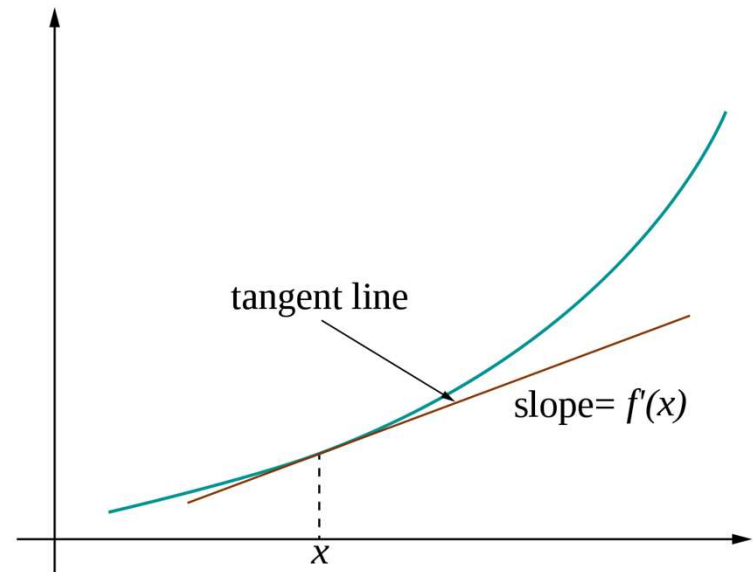
Previously: Functions

- A function is a process f that associates to each element x of a set X a single element $y = f(x)$ from a set Y .
- Example:

$$\begin{aligned} f: \mathbb{R} \setminus \{2\} &\longrightarrow \mathbb{R} \\ x &\longmapsto \frac{3x^2 + 2}{x - 2} \end{aligned}$$

Derivative

- The derivative of a function at a point is the slope of the tangent line to the graph of the function at that point.
- It represents the “rate of change” of the function.
 - Example: the derivative of an object position relative to the time is the object’s velocity
- The derivative of a function f is noted f'



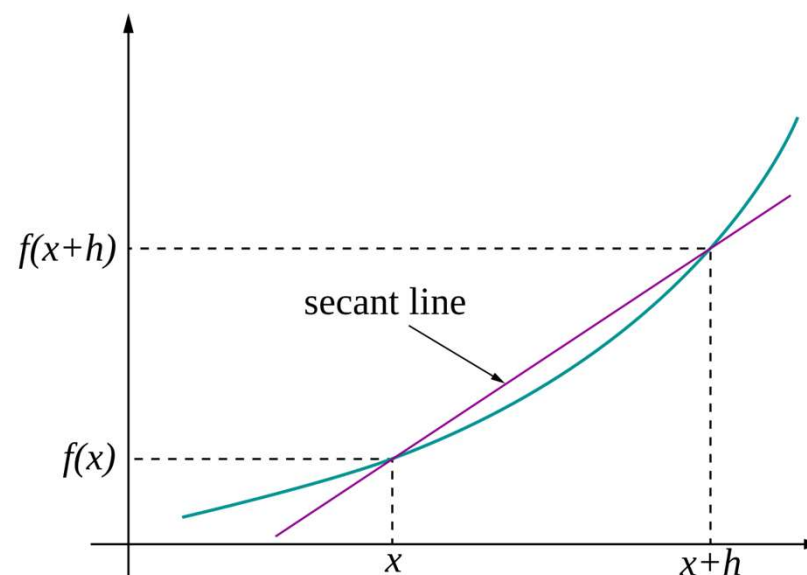
Differentiation

- Action of computing a derivate
- The slope of a line between two points of the graph of a function f is:

$$\frac{f(x+h) - f(x)}{h}$$

- When h is small, this expression approaches the derivative:

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$



Examples

$$f(x) = x \implies f'(x) = 1$$

$$f(x) = x^2 \implies f'(x) = 2x$$

$$f(x) = x^3 \implies f'(x) = 3x^2$$

$$f(x) = 1/x \implies f'(x) = -1/x^2$$

$$f(x) = e^x \implies f'(x) = e^x$$

$$f(x) = \sin(x) \implies f'(x) = \cos(x)$$

$$f(x) = \cos(x) \implies f'(x) = -\sin(x)$$

Higher derivatives

- The derivative of f' is written f''
- It is called the second derivative of f
- If $f(t)$ is the position of an object at time t
 - $f'(t)$ is the object's velocity
 - $f''(t)$ is the object's acceleration

Approximating a derivate

- If f is unknown, but we know some of its values, we can approximate its derivative:

- Forward rate:

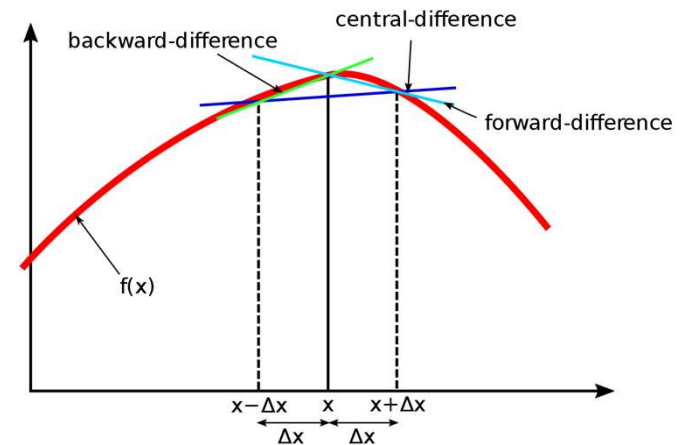
$$\frac{f(x+h) - f(x)}{h}$$

- Backward rate:

$$\frac{f(x) - f(x-h)}{h}$$

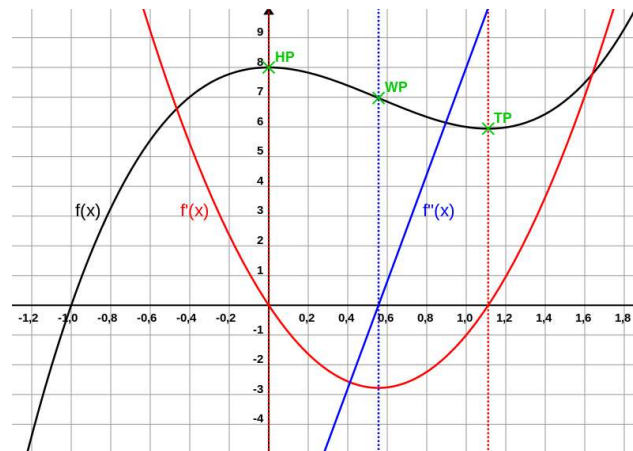
- Central rate:

$$\frac{f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right)}{h}$$



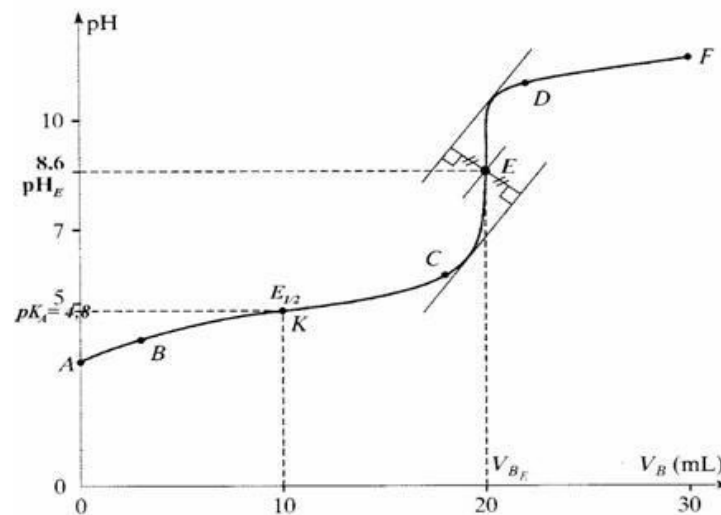
Special points

- A stationary point is a point where the derivative is zero
 - It is a turning point if the derivative also and changes sign
- An inflection point is a point where the second derivative is zero and changes sign



109titration

- Acid-base titration: find the concentration of an acid (or a base) by adding progressively a standard solution of base (or acid) with a known concentration and reading the pH.
- The initial concentration is deduced from the equivalence point



109titration

- Goal: use derivative approximations to find the equivalence point of an acid-base titration
- Input: csv file with vol;ph points
- Outputs:
 - First derivative values
 - Equivalence point estimated from the first derivate
 - Second derivative values
 - Approximation of the second derivative values every 0.1 ml around the estimated equivalence point
 - Better estimation of the equivalence point from the second derivative

Exercise: Rate of change

- The rate of change between two points $(x_0, f(x_0))$ and $(x_1, f(x_1))$ is
$$\frac{f(x_1) - f(x_0)}{x_1 - x_0}$$
- Create a function that takes two points $(x_0, f(x_0))$ and $(x_1, f(x_1))$ and returns the rate of change between those points

Exercise: Derivative estimation

- In this project, the derivative is approximated by computing the weighted mean of the backward rate and the forward rate.
 - The weighted mean of x and y with weights a and b is
$$\frac{ax + by}{a + b}$$
 - What weights should you use for the rates?
- Create a function that takes three points $(x_0, f(x_0))$, $(x_1, f(x_1))$ and $(x_2, f(x_2))$ and returns an estimation of the derivative $f'(x_1)$

Exercise: Linear approximation

- Since a function can be approximated by a line between two close points, we can also estimate the value of the function for any point between these two.
- Create a function that takes two points $(x_0, f(x_0))$ and $(x_1, f(x_1))$, a value x , and returns an estimation of $f(x)$.