109titration

B-MAT-200

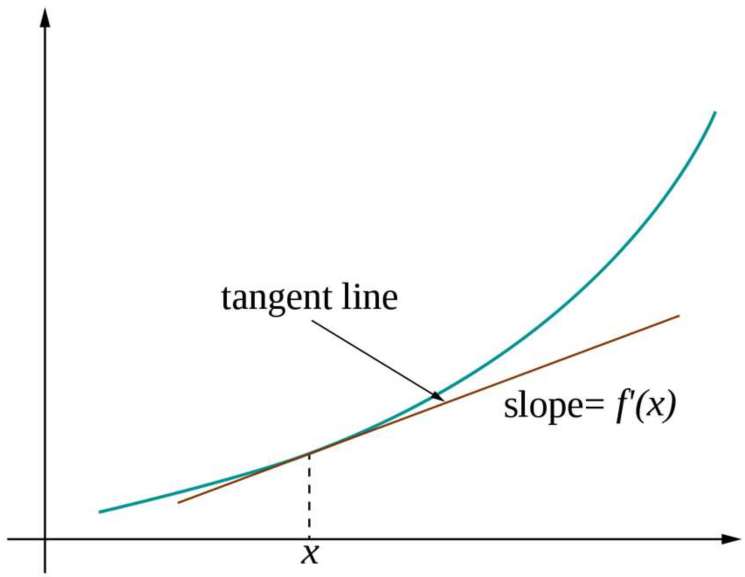
Previously: Functions

- 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:

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

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'



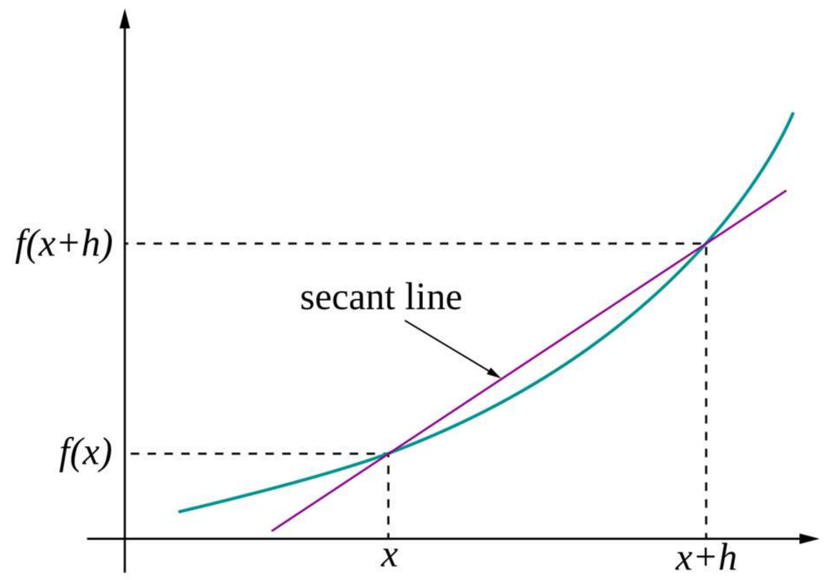
Differentiation

- 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:

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



Examples

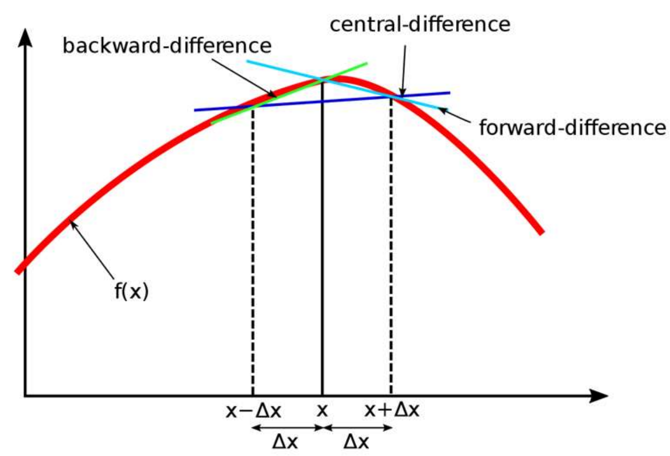
$$
\begin{aligned}
f(x) = x &\Longrightarrow f'(x) = 1 \\
f(x) = x^2 &\Longrightarrow f'(x) = 2x \\
f(x) = x^3 &\Longrightarrow f'(x) = 3x^2 \\
f(x) = 1/x &\Longrightarrow f'(x) = -1/x^2 \\
f(x) = e^x &\Longrightarrow f'(x) = e^x \\
f(x) = \sin(x) &\Longrightarrow f'(x) = \cos(x) \\
f(x) = \cos(x) &\Longrightarrow f'(x) = -\sin(x)
\end{aligned}
$$

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

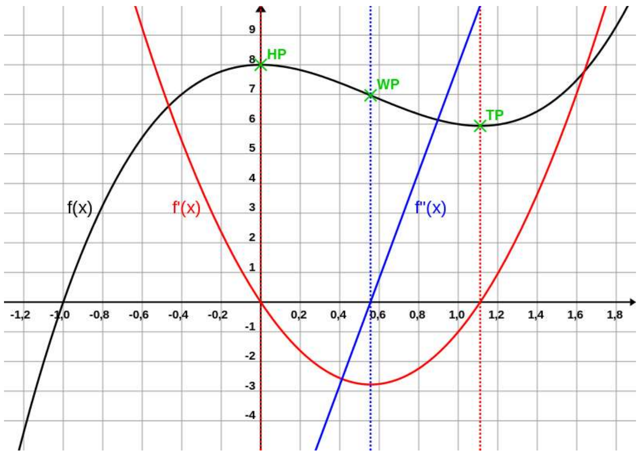
Approximating a derivate

- 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



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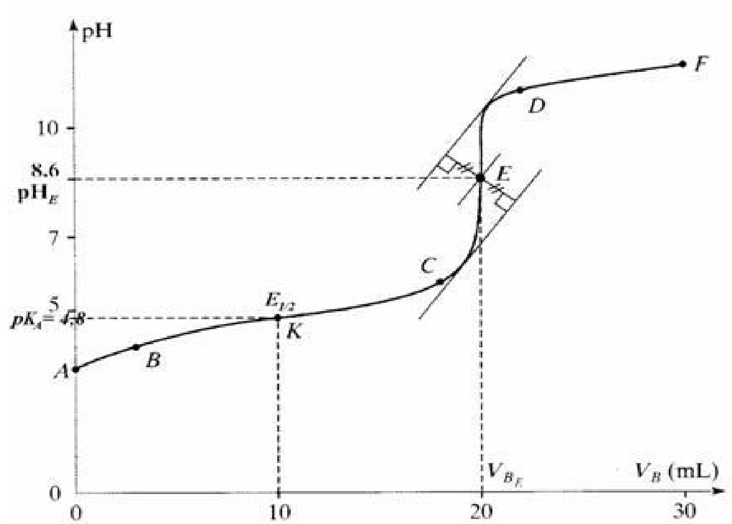
- Acid-base titration: find the concentration of an acid (or a base) by adding progressively a standard solution of base (or acid) with a known concentration and reading the pH.
- The initial concentration is deduced from the equivalence point



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- 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 $\left(x_0, f(x_0)\right)$ and $\left(x_1, f(x_1)\right)$ 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 $\frac{ax+b}{a+b}$
  - 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 $f(x)$.