Mathematical background of Physical Chemistry I

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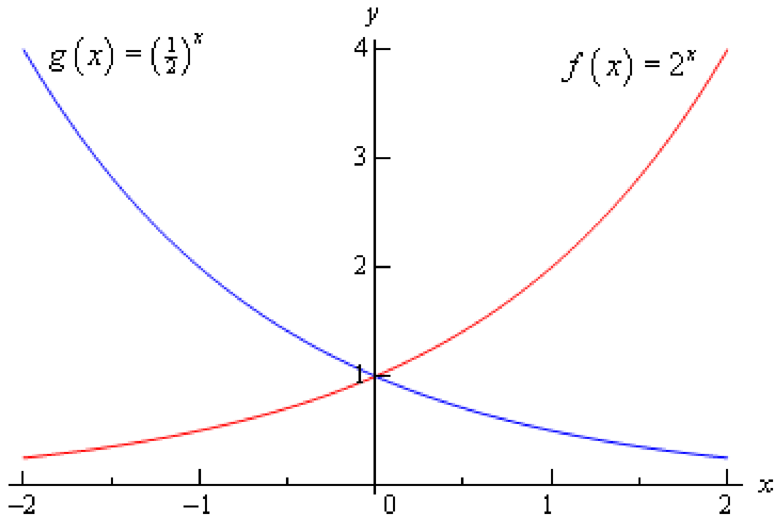
Exponential functions

- $2^n = 2 \times 2 \times 2 \times \cdots \times 2$
- $2^{n/m} = \sqrt[m]{2^n}$
- $2^{-n/m} = \dfrac{1}{2^{n/m}}$



- $e = \lim_{n\to\infty}(1 + \frac{1}{n})^n = 1 + \frac{1}{1!} + \frac{1}{2!} + \frac{1}{3!} + \ldots$, where

  $e = 2.718281828459045235360287471352662497757247093699995$

- Expression 'exponential function' generally refers to e^x

  $e^x = \lim_{n\to\infty}(1 + \frac{x}{n})^n = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$

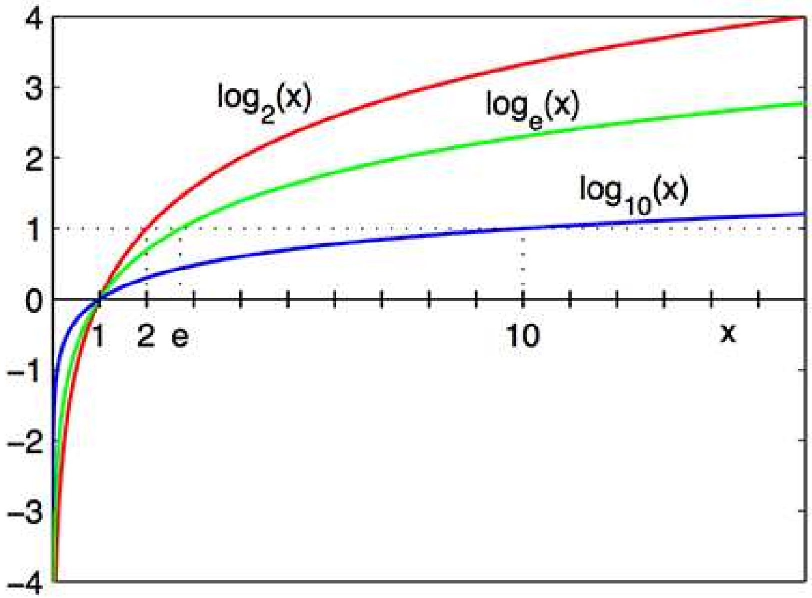
Logarithm

- Inverse of a function: $g(x) = f^{-1}(x)$ if $g(f(x)) = x$.

- The logarithm is the inverse operation to exponentiation, e.g., $2^{\log_2 x} = x$.

- $\log_2 8 =$ *How many 2s do we multiply to get 8?*

- Plots of logarithm functions:



- Properties of logarithm:

log of product	$\log_a(xy) = \log_a(x) + \log_a(y)$
log of fraction	$\log_a(x/y) = \log_a(x) - \log_a(y)$
log of exponential	$\log_a(x^y) = y \log_a(x)$
change the base of log	$\log_a(x) = \frac{\log_b(x)}{\log_b(a)}$

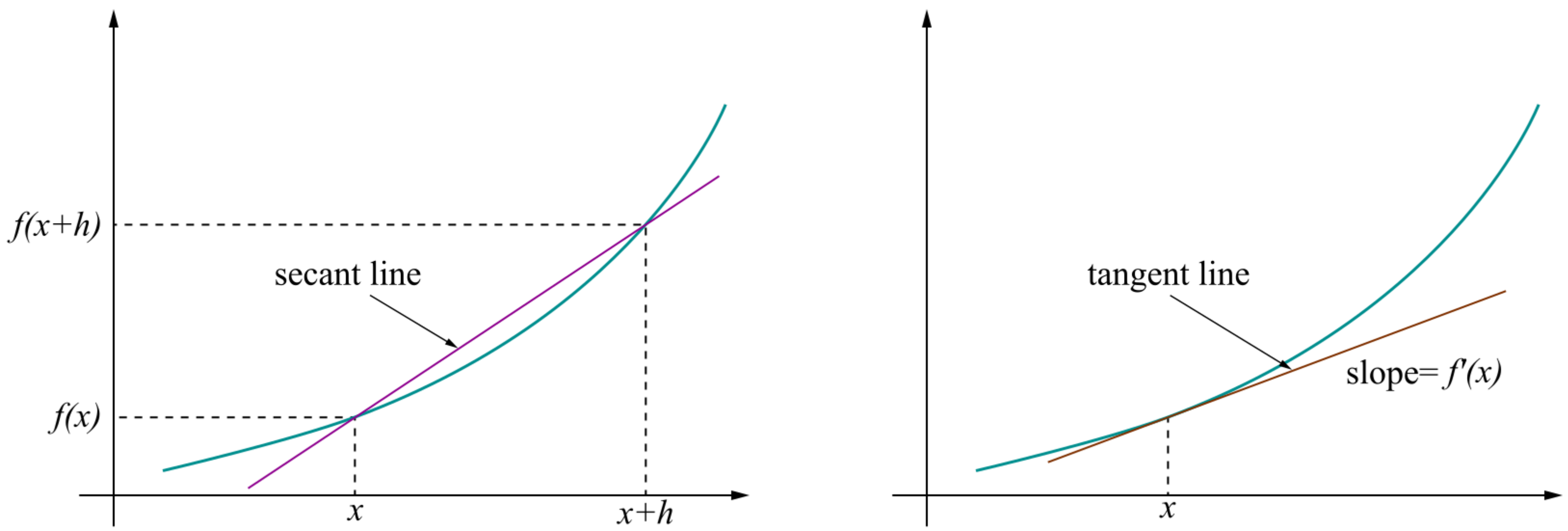
Sigma and Pi notation

- $\sum$ compactly represents summation of many similar terms: $\sum_i a_i$
- Π is frequently used for product of terms: $\Pi_i a_i$
- Examples
  - $\displaystyle\sum_{i=1}^{n} \ln(a_i) = \ln(a_1) + \ln(a_2) + \cdots + \ln(a_n)$
    $\displaystyle= \ln(a_1 a_2 \ldots a_n) = \ln(\prod_{i=1}^{n} a_i)$
  - $\displaystyle e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

Derivation of single-variable functions

- The derivative of a function of a real variable measures the sensitivity to change of the function value (output value) with respect to a change in its argument (input value).

- $f'(x) = f^{(1)}(x) = \dfrac{df(x)}{dx} = \lim_{h \to 0} \dfrac{f(x+h) - f(x)}{h}$



- Derivatives of simple functions

$f(x)$	$f'(x)$	$f(x)$	$f'(x)$
$const$	0	$\ln x$	$1/x$
x^2	$2x$	$\sin x$	$\cos x$
$\sqrt{x}$	$0.5x^{-0.5}$	$\cos x$	$-\sin x$
x^n	nx^{n-1}	e^x	e^x

- Derivation of combined functions

linearity $(af(x) + bg(x))' = af(x)' + bg(x)'$

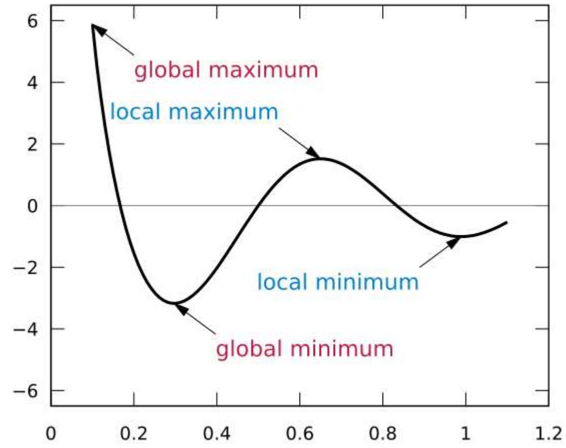
product rule $(f(x)g(x))' = f(x)'g(x) + f(x)g(x)'$

quotient rule $\left(\frac{f(x)}{g(x)}\right)' = \frac{f(x)'g(x) - f(x)g(x)'}{g(x)^2}$

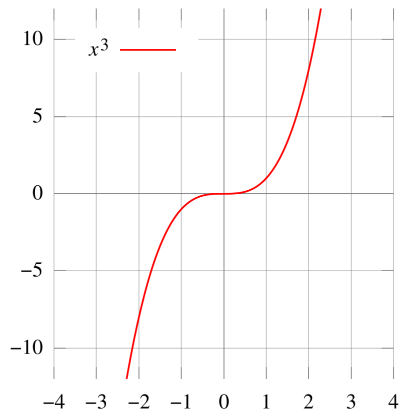
chain rule $f\,(g(x))' = \frac{df(g(x))}{dg(x)}\frac{dg(x)}{dx}$

Second derivatives

- At local minima and maxima of a function the slope is zero: $f'(x_0) = 0$
- If the second derivative, $f''(x_0) > 0$, is positive at x_0 it is a minima, if $f''(x_0) < 0$ it is a maxima. If $f''(x_0) = 0$ the higher derivatives should be investigated (e.g. $f(x) = x^4$ at $x = 0$).



- In general, if $f''(x) > 0$ the tangent 'below' the function, if $f''(x) < 0$ it is 'above' the curve. If $f''(x_0) = 0$ (and $f'''(x_0) \neq 0$), x_0 can be an inflection point (e.g. $f(x) = x^3$ at $x = 0$).



Snowdrop (Hóvirág)

Taylor-series

- Polynomial approximation of a function:

  $f(x) = f(x_0) + \frac{1}{1!}f^{(1)}(x_0)(x - x_0) + \frac{1}{2!}f^{(2)}(x_0)(x - x_0)^2 +$
  $\frac{1}{3!}f^{(3)}(x_0)(x - x_0)^3 + \frac{1}{4!}f^{(4)}(x_0)(x - x_0)^4 + \ldots,$

  where $f^{(n)}(x) = \frac{d^n f}{dx^n}$.

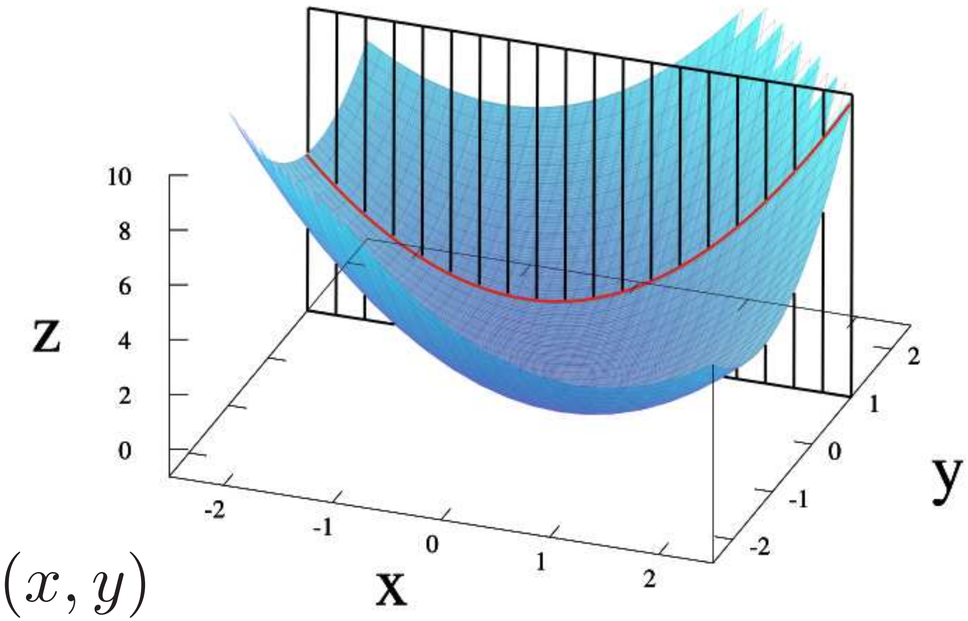
- Linear approximation: $\Delta f \approx \frac{df}{dx}|_{x=x_0}\Delta x$

  ($\Delta x = (x - x_0)$ and $\Delta f = f(x) - f(x_0)$).

- If Δx is infinitesimal, than Δx^2 is considered to be zero, and $df = \frac{df}{dx}dx$. It is the differential of $f(x)$.

- Taylor-series: $f(x) = \displaystyle\sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x_0)(x - x_0)^n$

Partial derivative



- $z = f = f(x, y)$ defines a surface.

- $\frac{\partial f(x,y)}{\partial x}$, $\frac{\partial f(x,y)}{\partial y}$: the task is to find the slope of a two-variable (or multi-variable) function in the directions of x and y.

- Definition: $$\left.\frac{\partial f}{\partial x}\right|_y = \lim_{h\to 0}\frac{f(x+h,y)-f(x,y)}{h},$$ $$\left.\frac{\partial f}{\partial y}\right|_x = \lim_{h\to 0}\frac{f(x,y+h)-f(x,y)}{h}$$

- For continuous, well-behaving functions: $\frac{\partial}{\partial y}\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}\frac{\partial f}{\partial y}$ (Young-theorem)

Exact differential

- Linear approximation of a function of two variables:

  $$\Delta f \approx \left.\frac{\partial f}{\partial x}\right|_{x,y=x_0,y_0} \Delta x + \left.\frac{\partial f}{\partial y}\right|_{x,y=x_0,y_0} \Delta y.$$

- The higher order terms contain contributions proportional to Δx^2, Δy^2, $\Delta x \Delta y$, $\Delta x \Delta y^2$ *etc.*

- If Δx and Δy are infinitesimal, than $df = \left.\frac{\partial f}{\partial x}\right|_y dx + \left.\frac{\partial f}{\partial y}\right|_x dy.$

  It is called the exact differential of $f(x, y)$.

Indefinite integral

- Reverse of differentiation: if $\frac{dF(x)}{dx} = f(x)$ than $\int f(x)dx = F(x) + C$, where $F(x)$ is the indefinite integral of $f(x)$ and C is an arbitrary constant.

- Indefinite integral of elementary functions:

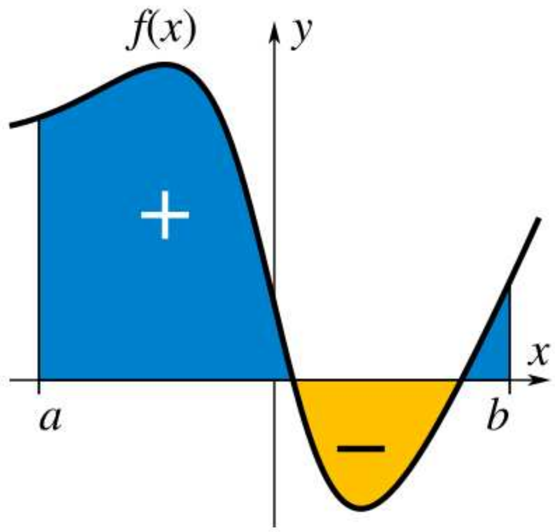
$f(x)$	$\int f(x)$	$f(x)$	$\int f(x)$
x^n	$\frac{x^{n+1}}{n+1}$	$\frac{1}{x}$	$ln\|x\|$
x	$x^2/2$	$\cos x$	$\sin x$
e^{ax}	$\frac{1}{a}e^{ax}$	$\sin x$	$-\cos x$
$\ln(x)$	$x(ln(x) - 1)$	c	cx

- Notation: $\int dx = \int 1dx$

Definite integral

- The signed area below (plus sign) or above (minus sign) the graph of function f in the interval bounded by a and b: $\int_a^b f(x)dx$.

- Newton-Leibnitz formula: $\int_a^b f(x)dx = [F(x)]_a^b = F(b) - F(a)$, where $F(x)$ is the indefinite integral of $f(x)$.



- To understand the N-L formula consider a short interval with length h: $hf(a) \approx \int_a^{a+h} f(x)dx = F(a+h) - F(a)$. If h goes to zero $f(a) = \frac{dF}{dx}|_{x=a}$.