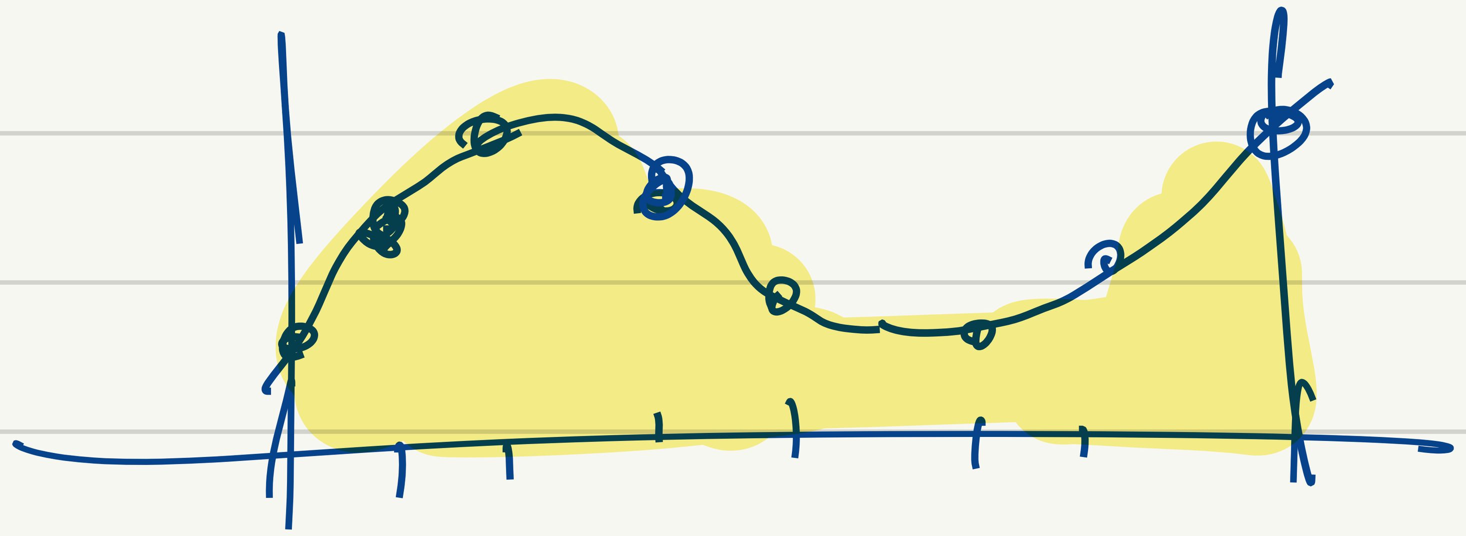
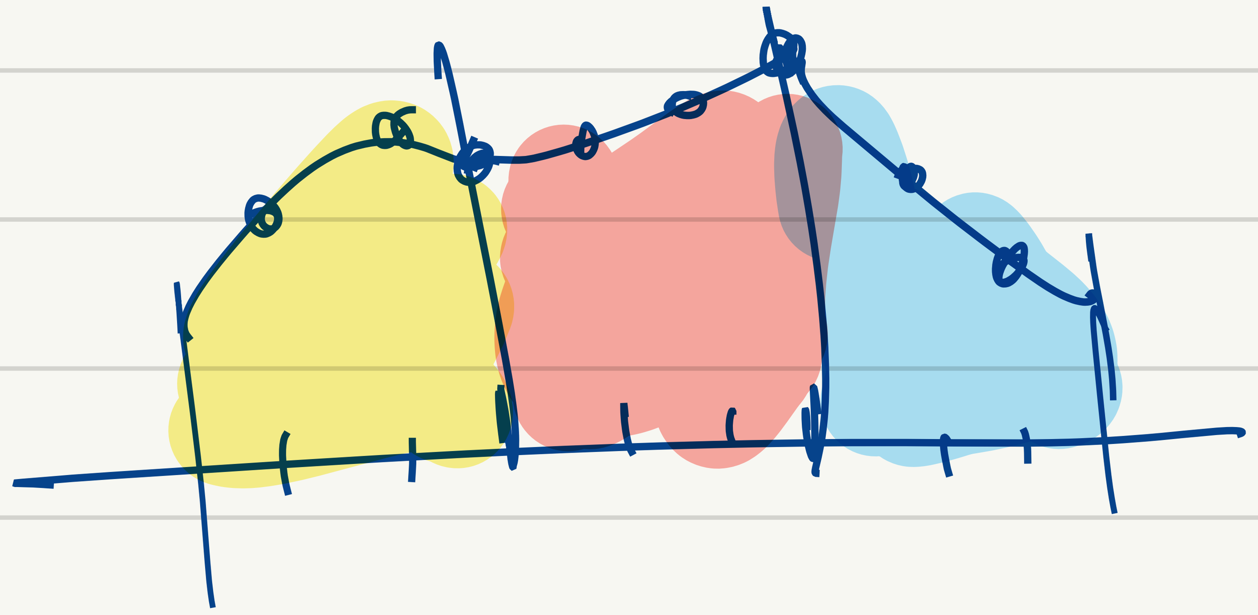
Numerical integration, differentiation, optimization

$f : \mathbb{R} \to \mathbb{R}$

$[a, b]$



Simple quadrature

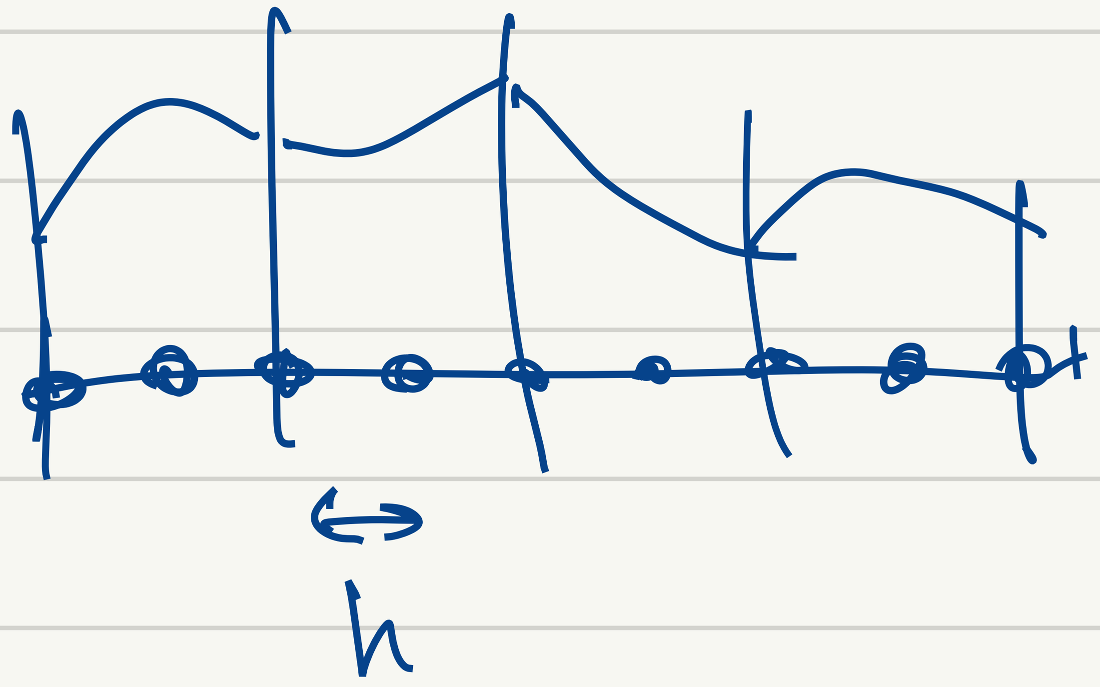


Composite quadrature

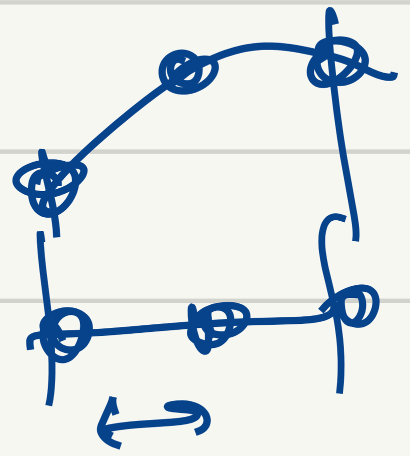
Divide $[a,b]$ into $\underline{k}$ pieces,
Apply some fixed quadrature rule $\underline{Q_n}$ on each

<u>Converges</u> as $k \to \infty$ as long as Q_n has degree ≥ 0

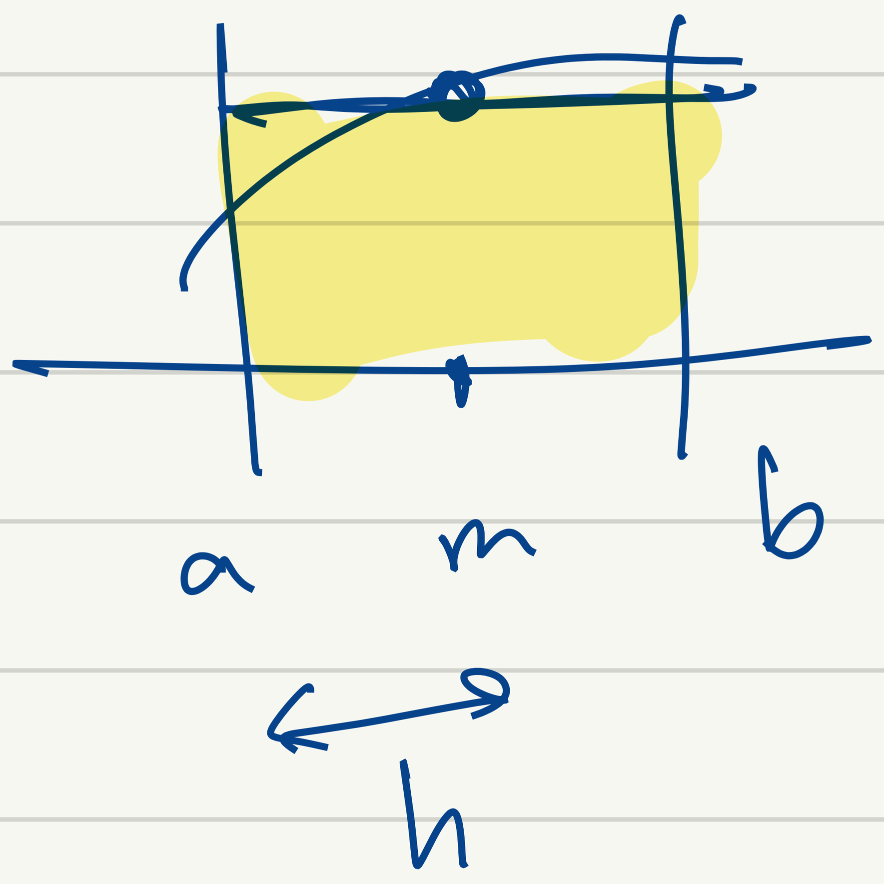
<u>Stable</u> if Q_n is stable



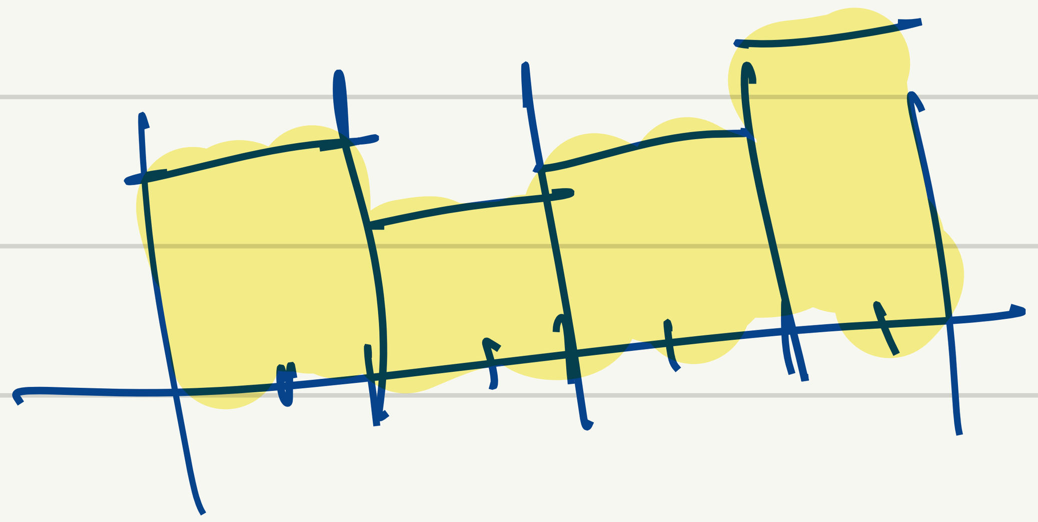
<u>Accuracy</u> as function of node spacing h



Composite midpoint:



Error in midpoint $= O\left((b-a)^3\right) = O(h^3)$



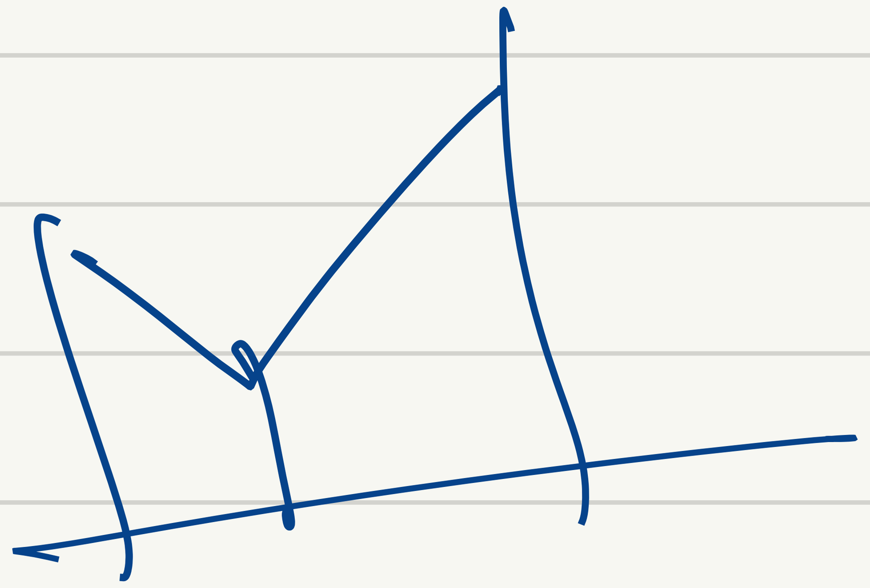
Error in composite midpoint

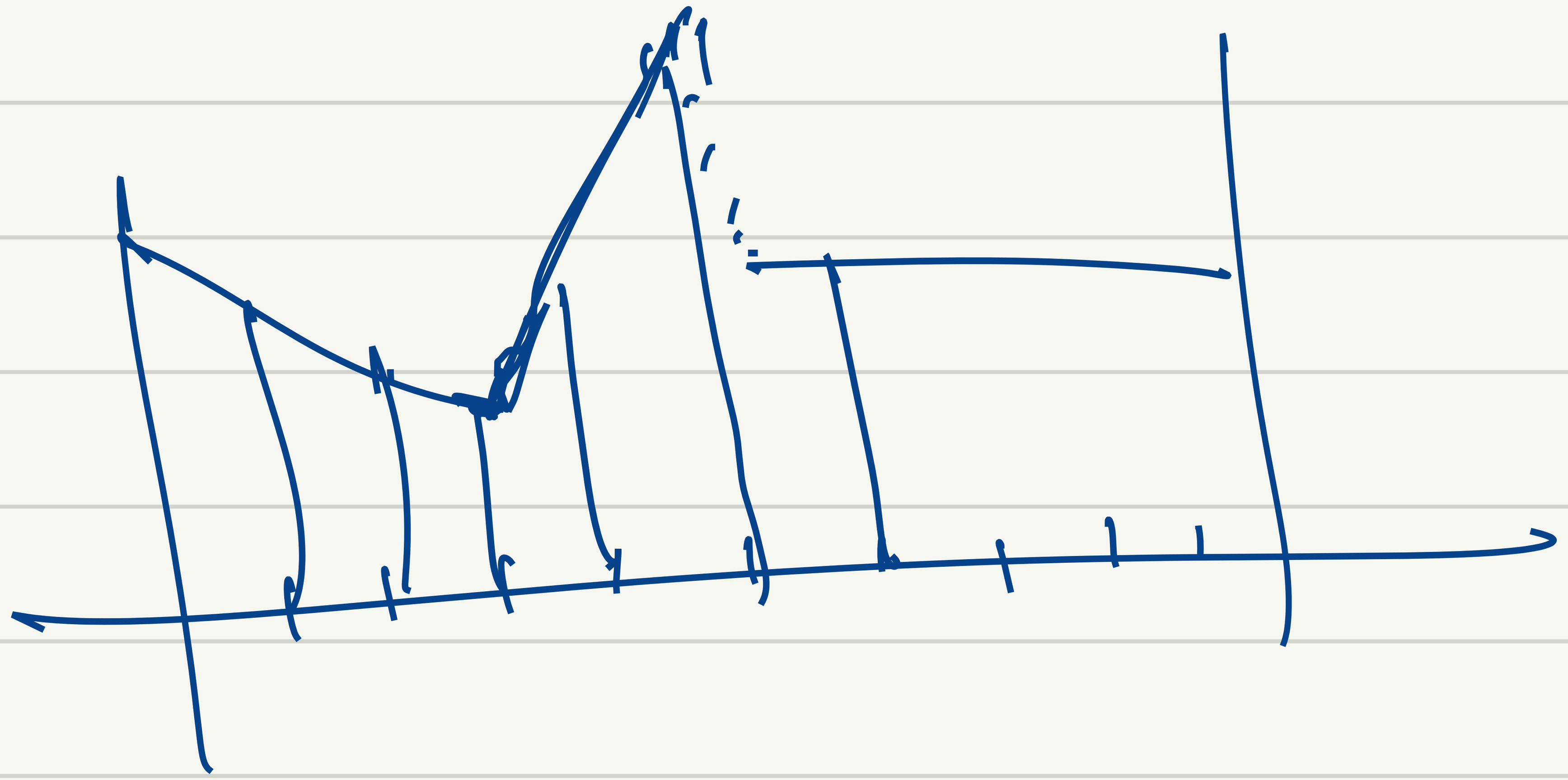
$$= \underbrace{\#\text{ pieces}}_{=k} \times \underbrace{\text{error per piece}}_{O(h^3)}$$

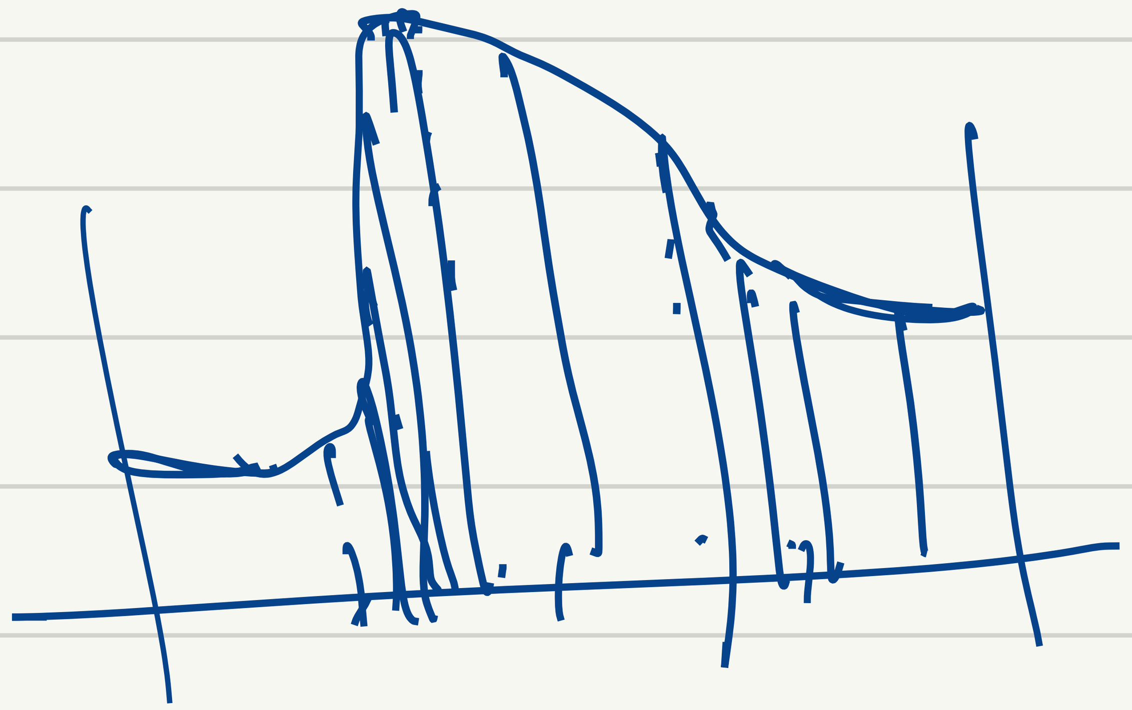
$$= O(k h^3) = O(h^2)$$: second-order accurate

Composite trapezoidal: 2nd order

" Simpson's rule: 4th order







Adaptive quadrature

Recursively subdivide pieces with high error

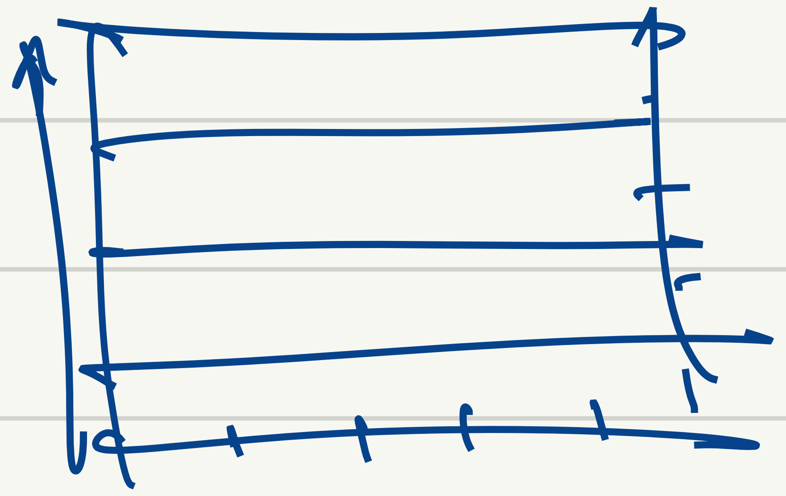
Error estimator:

1. $|Q_n(f) - Q_{2n}(f)|$
2. $|Q_n(f, [a,b]) - (Q_n(f,[a,m]) + Q_n(f,[m,b]))|$

Higher-dimensional integration

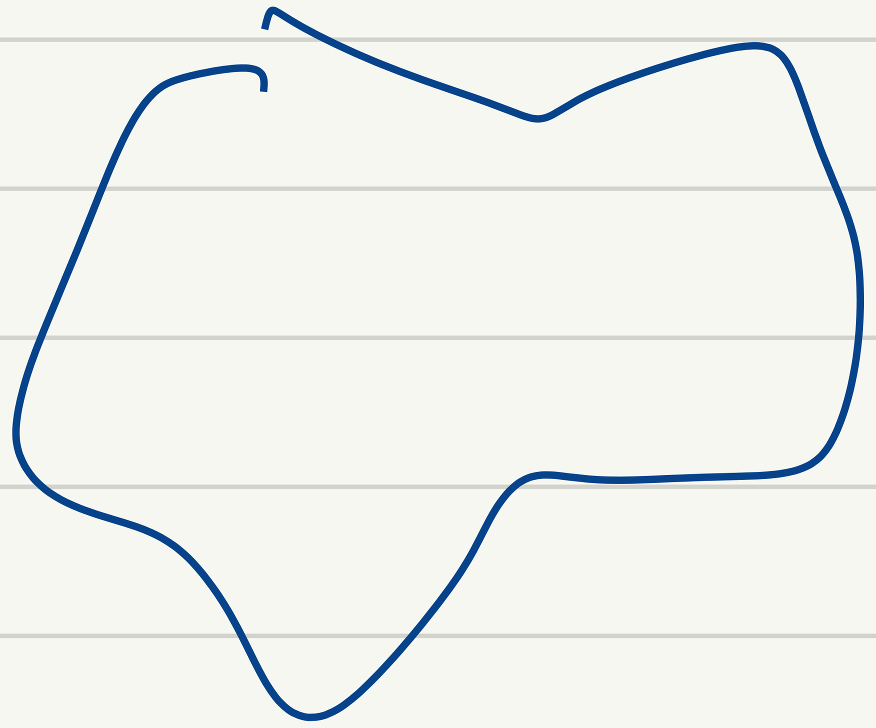
$f: \mathbb{R}^d \to \mathbb{R}$ over $\Omega \subseteq \mathbb{R}^d$

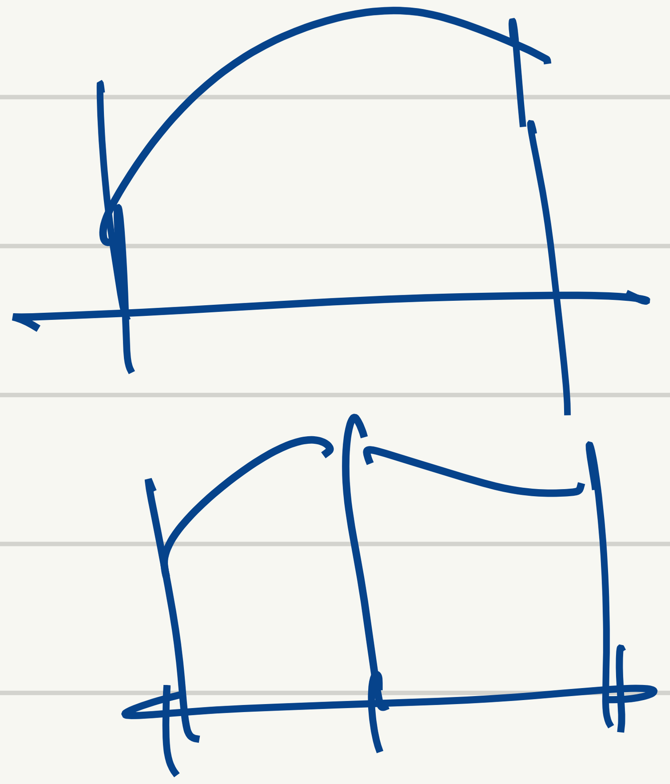
$$\iiint_\Omega f(x)\, dV$$



n

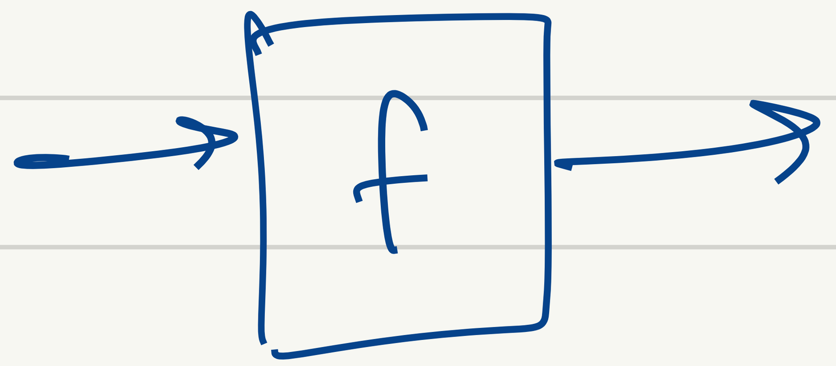
$$\underbrace{\int\left(\int f(x,y)\, dx\right) dy}$$





Large d → exponential # samples

Numerical differentiation

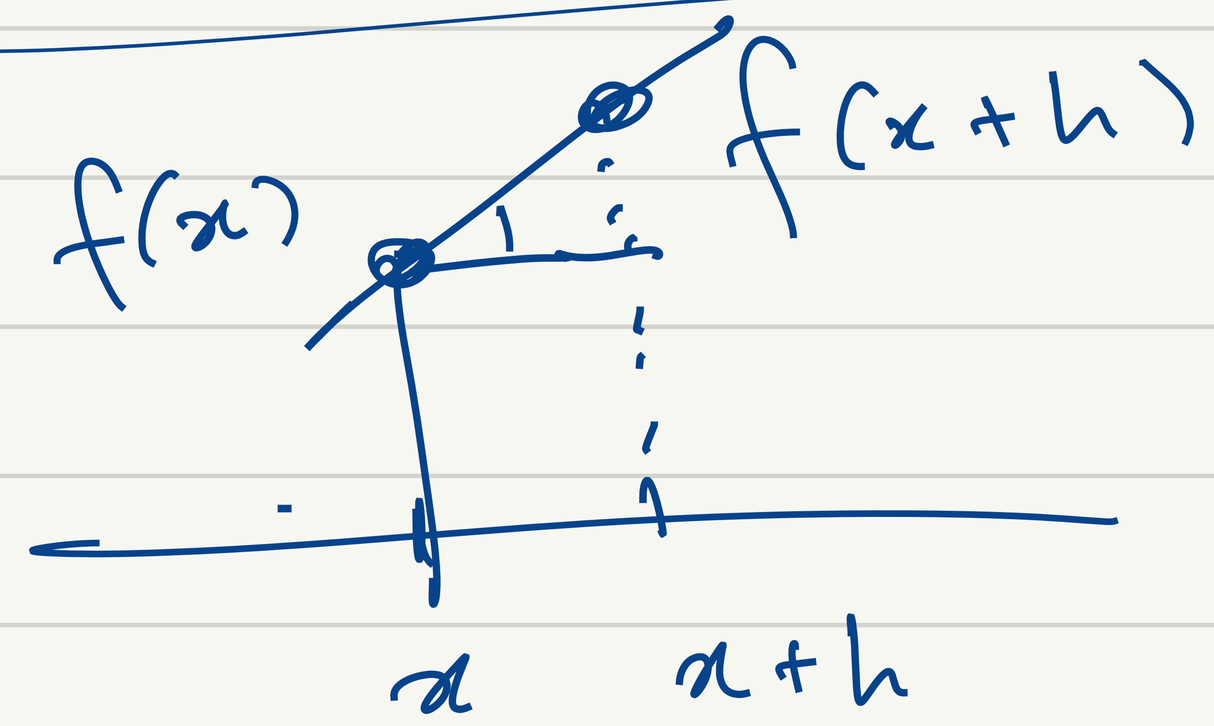


$$\frac{d^n f}{dx^n}$$

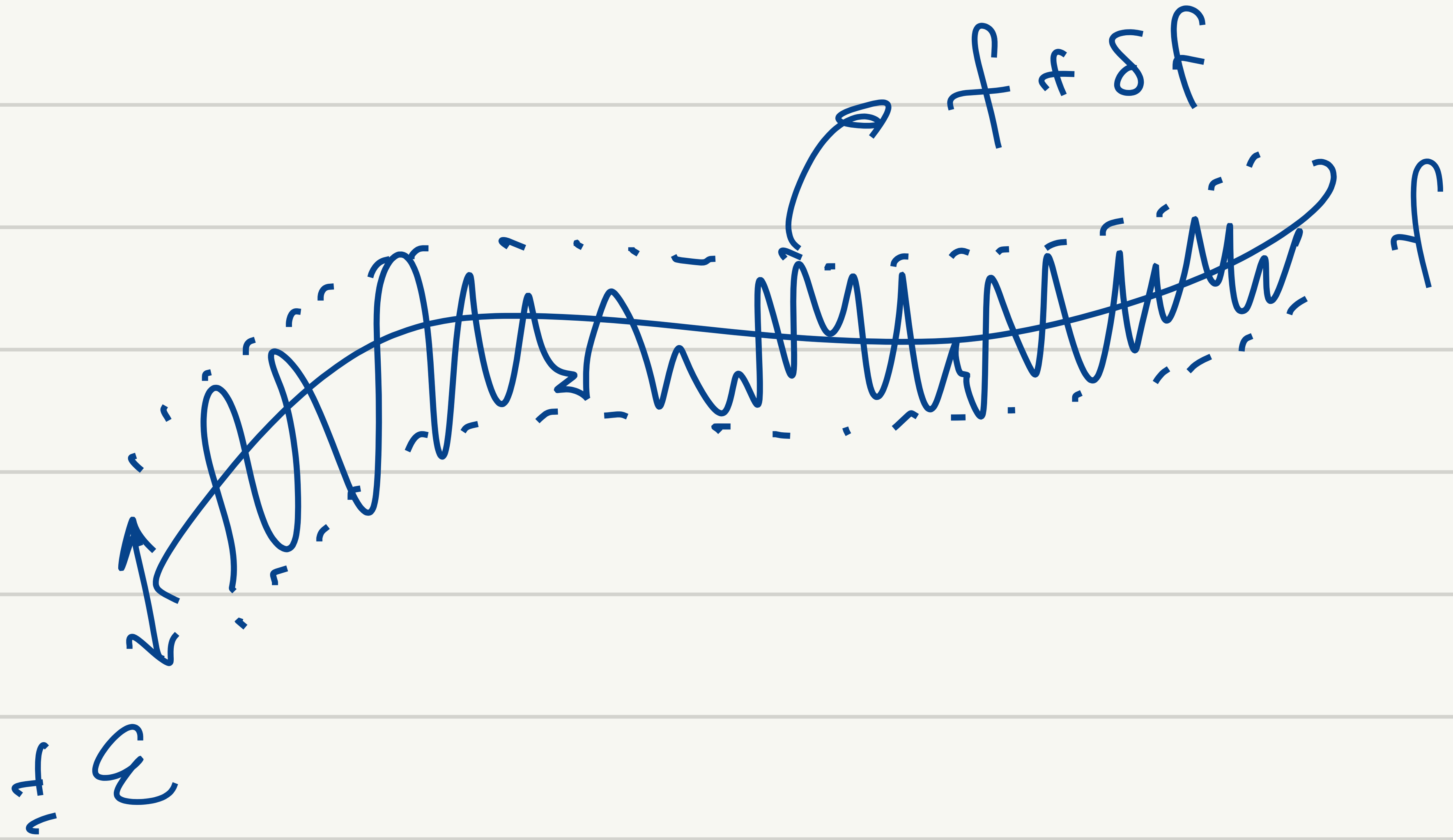
1. If f is black box / algorithm
2. If f' is too complicated
3. verify analytical derivative numerically

$$f \to f + \delta f, \quad \|\delta f\|_\infty \le \varepsilon$$

$$f' \to f' + \delta f', \quad \|\delta f'\|_\infty \le ?$$



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



$\boxed{\text{finite difference formulas}}$

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

$\boxed{\text{forward difference}}$

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

$\boxed{\text{backward difference}}$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \text{error}$$

Taylor series : $f(x+h) = \cancel{f(x)} + f'(x) \cdot h + \frac{f''(x)}{2!} h^2 + \frac{f'''(x)}{3!} h^3 + O(h^4)$

$$\Delta f(x) = \frac{1}{h}\left(f'(x) \cdot h + \frac{f''(x)}{2} h^2 + \frac{f'''(x)}{6} h^3 + \cdots \right)$$

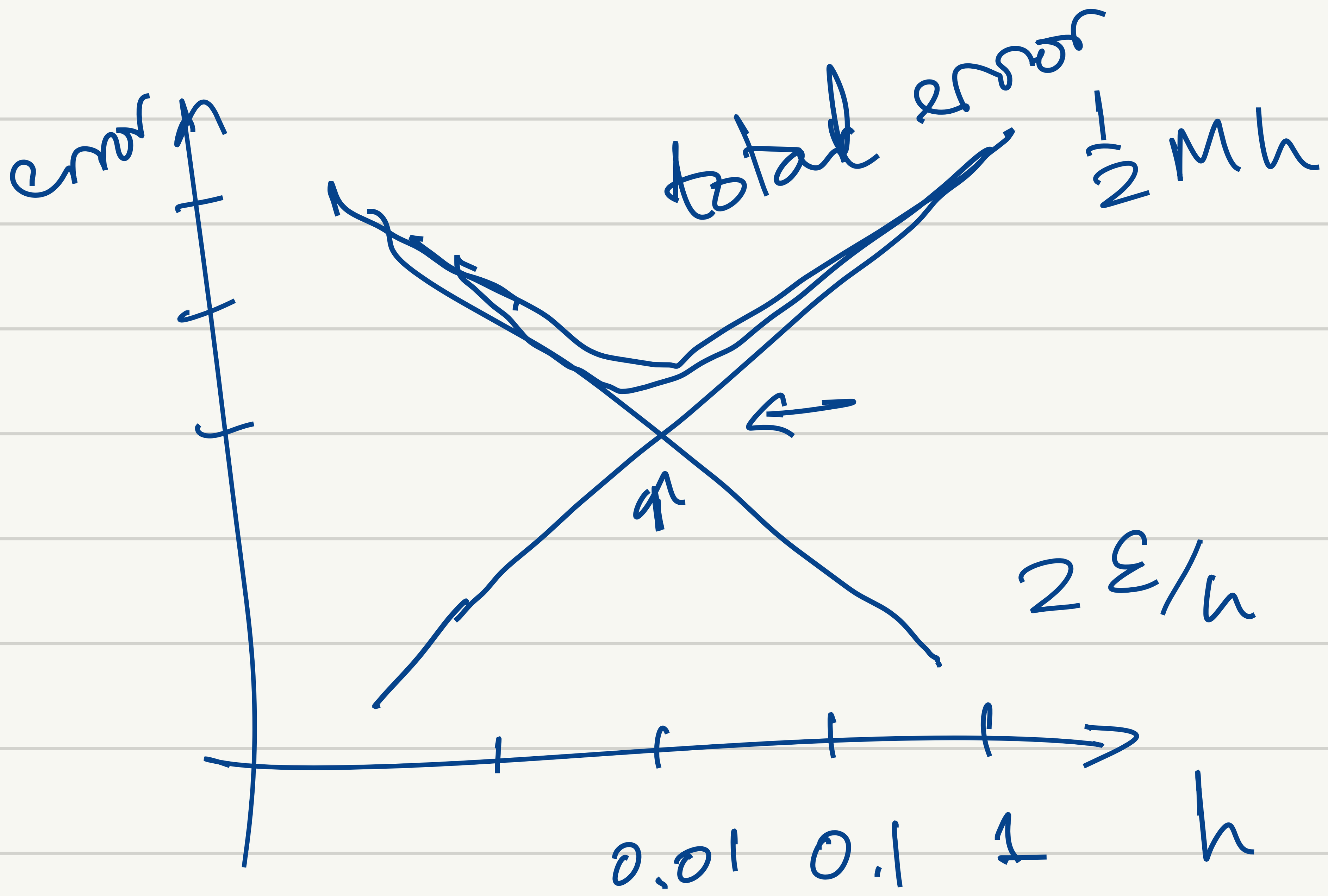
$$= \underbrace{f'(x)}_{\text{desired value}} + \underbrace{\tfrac{1}{2} f''(x) \cdot h + O(h^2)}_{\text{error} = O(h)}$$

forward diff. is 1st-order accurate.

same for backward diff.

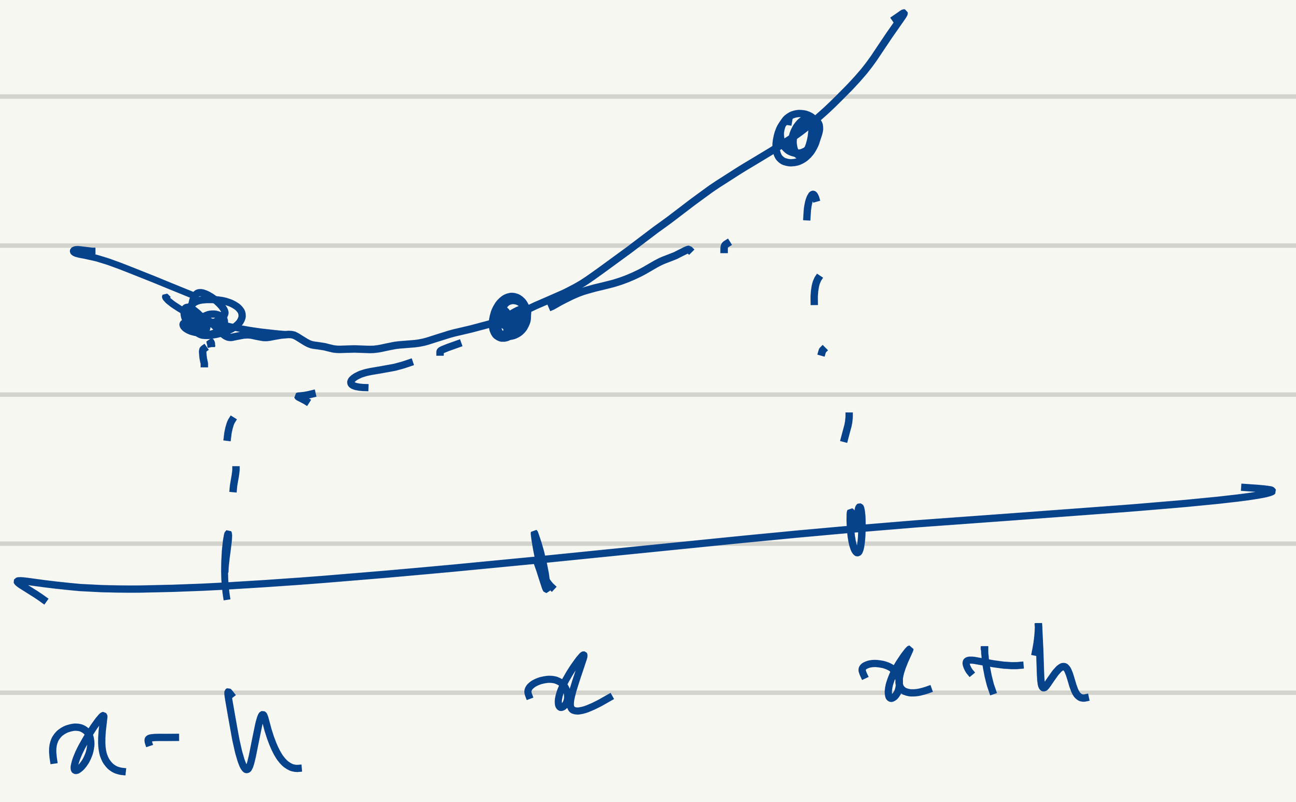
$|f''(x)| \leq M$, $|\tilde{f}(x) - f(x)| \leq \varepsilon$

$\Rightarrow |\Delta f(x) - f'(x)|$ involves truncation error $\frac{1}{2} M h$ and evaluation error $2\varepsilon/h$



$$\underbrace{\tfrac{1}{2}Mh, \qquad 2\varepsilon/h}$$

min at $h = O(\sqrt{\varepsilon/M})$

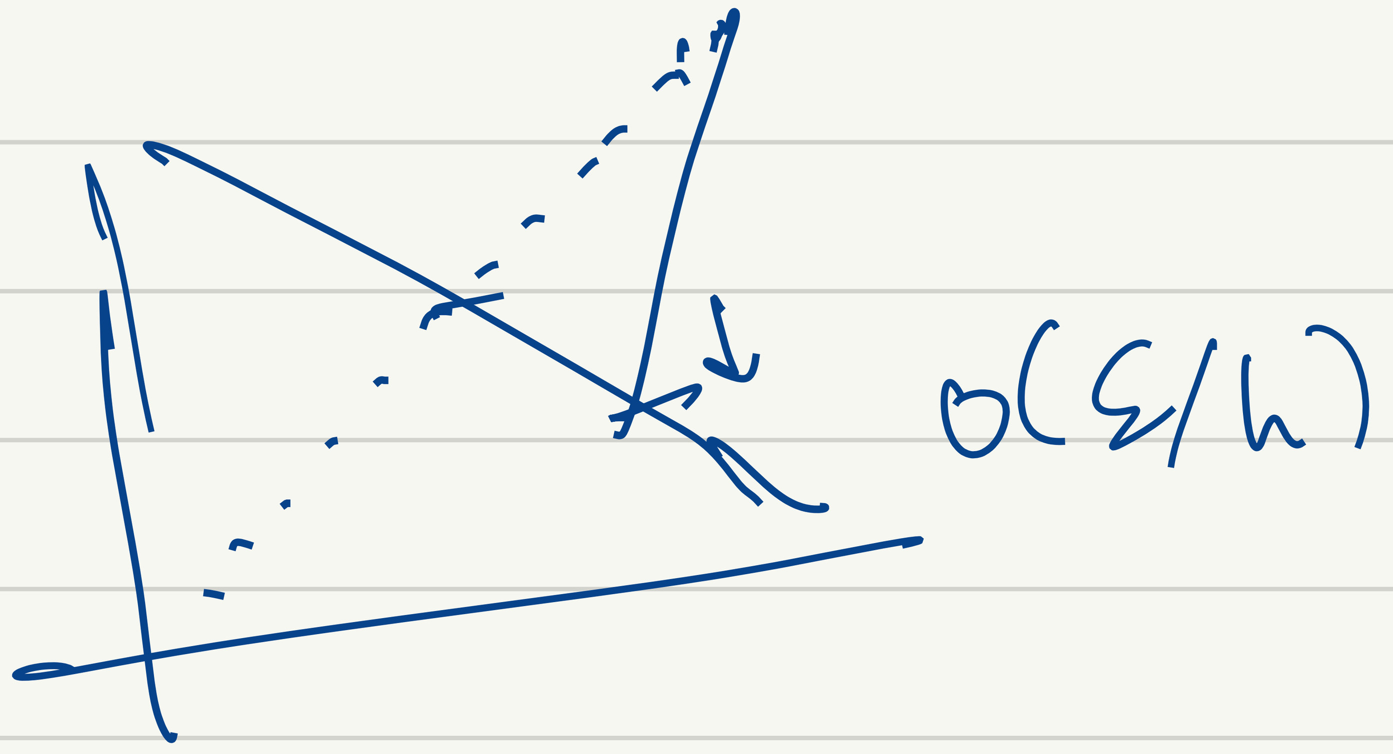


$f(x-h),\ f(x),\ f(x+h)$

$\boxed{\text{centered difference}}$

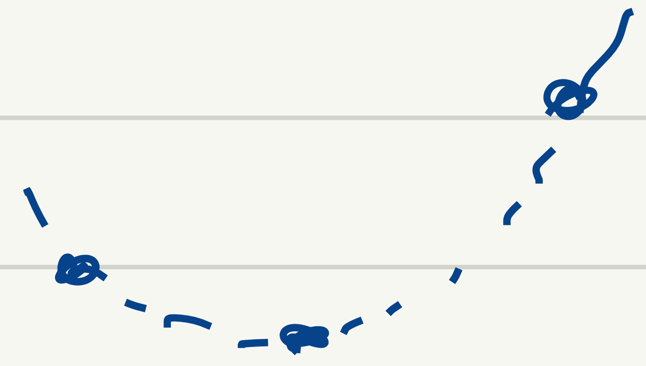
fit quadratic $p(x)$

$$f'(x) \approx p'(x) = \frac{f(x+h) - f(x-h)}{2h}$$



Error is $O(h^2)$: 2nd order

$f''(x)$: $f(x-h)$, $f(x)$, $f(x+h)$



$$f''(x) \approx p''(x) = \frac{f(x+h)+f(x-h)-2f(x)}{h^2}$$

centered diff., 2nd order

<u>Richardson extrapolation</u> : $F(h) = a + \cancel{O(h^p)}$

numerical scheme

correct answer

Optimization

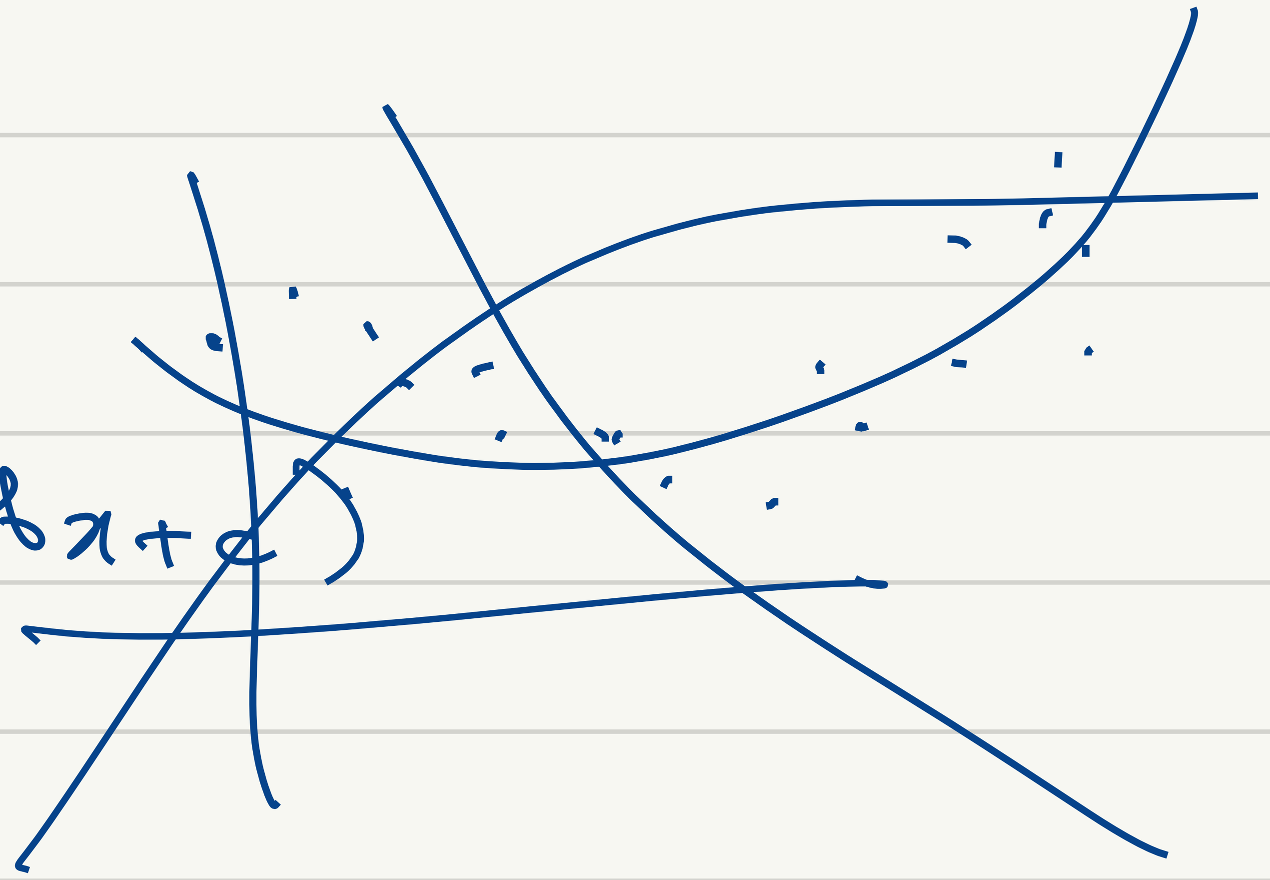
$f: S \to \mathbb{R}$ $\quad \boxed{\text{objective function}}$

find $x \in S$ s.t. $f(x) \le f(y) \ \forall y \in S$

(or $f(x) \ge f(y)$)

Data fitting / machine learning : choose parameters (a,b,c) of model (eg. ax^2+bx+c)

to min. error w.r.t. data

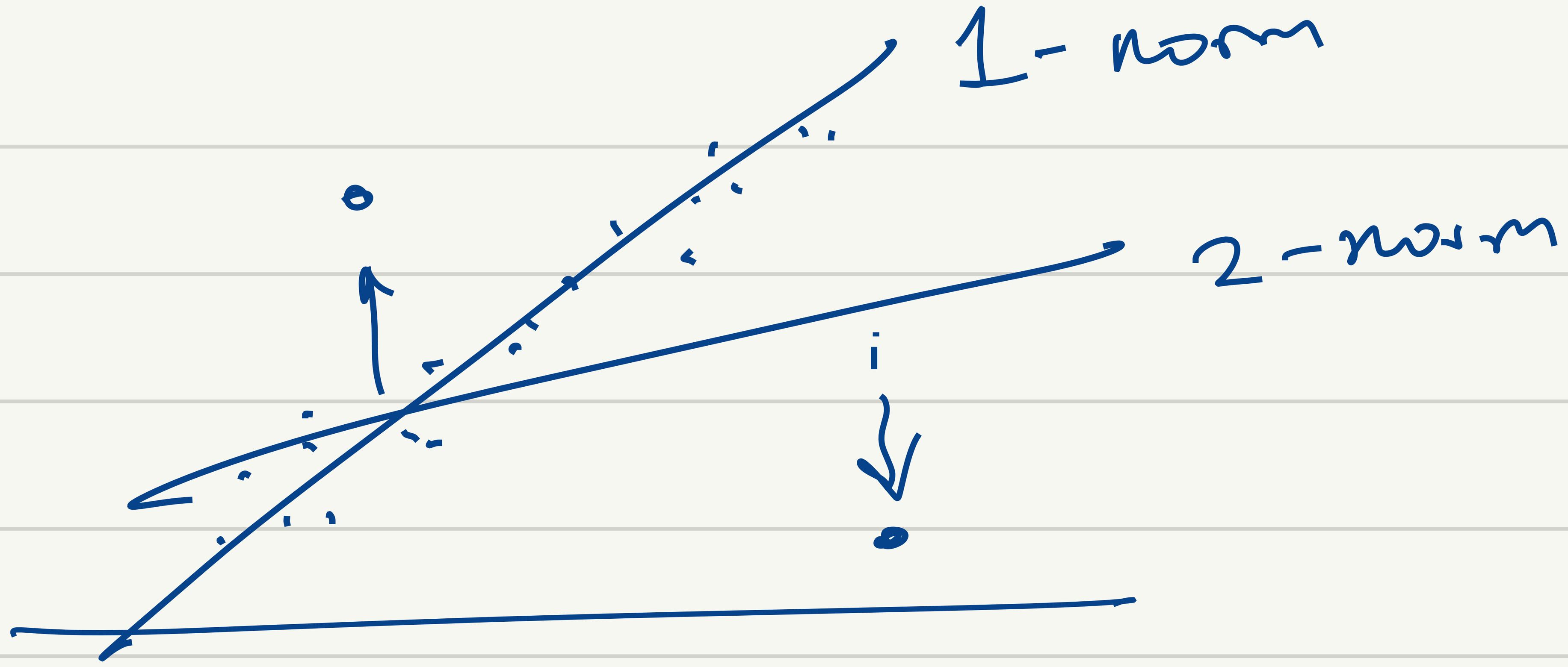


least squares : model is linear ($y = Ax$), obj. was 2-norm

($\min \|y - Ax\|_2$)

$\min \|y - Ax\|$ eg: 1-norm $\sum |y_i - (Ax)_i|$

∞-norm : $\max |y_i - (Ax)_i|$



Optimization problems

find $x \in S$

to minimize $f(x)$

discrete ✗

continuous

$S \subseteq \mathbb{R}^n$

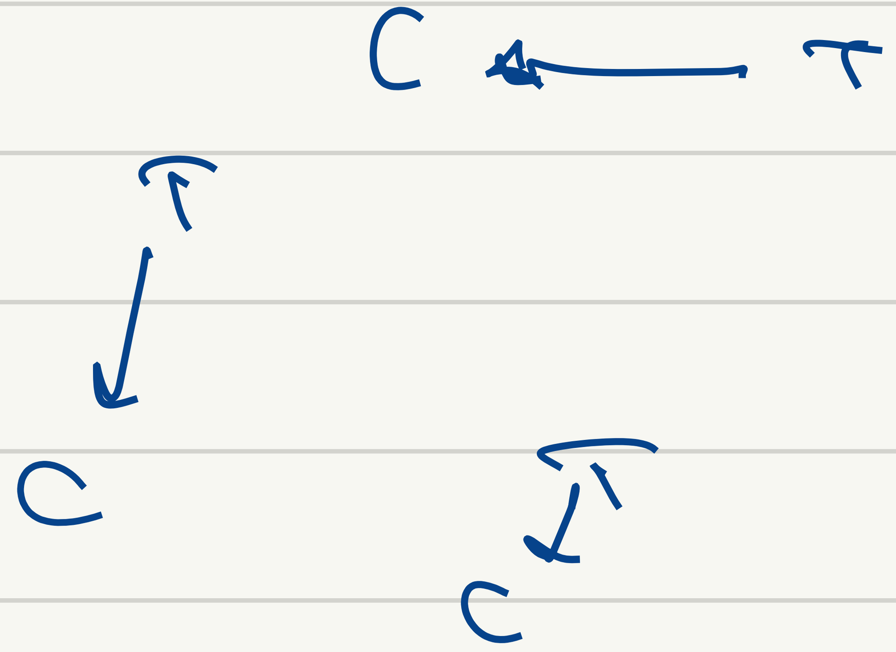
f continuous

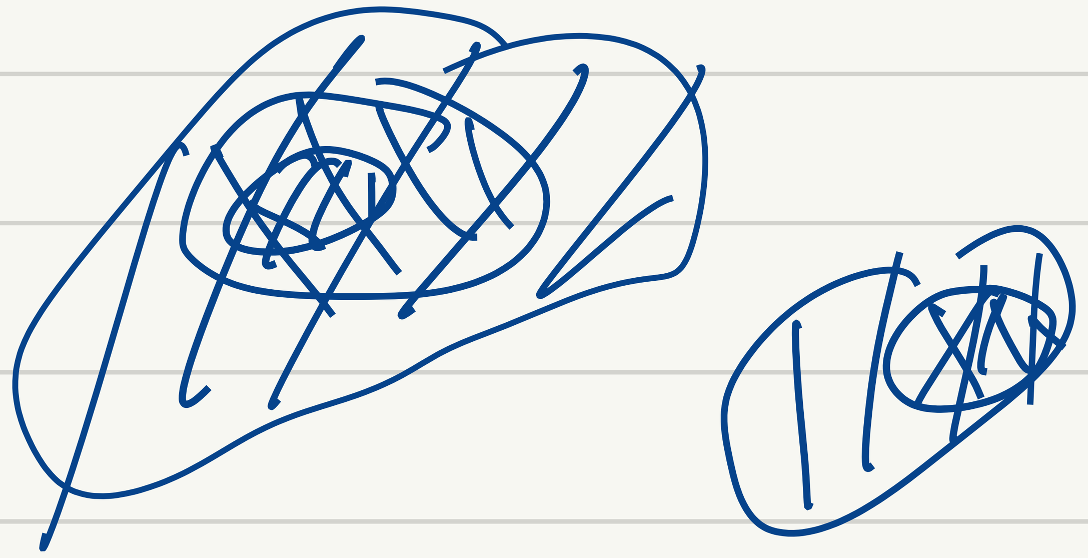
✓ unconstrained

$S = \mathbb{R}^n$

constrained ✗

$S \subset \mathbb{R}^n$





x_i : money to spend on component i

$x_i \geq 0$. $\sum x_i \leq$ budget

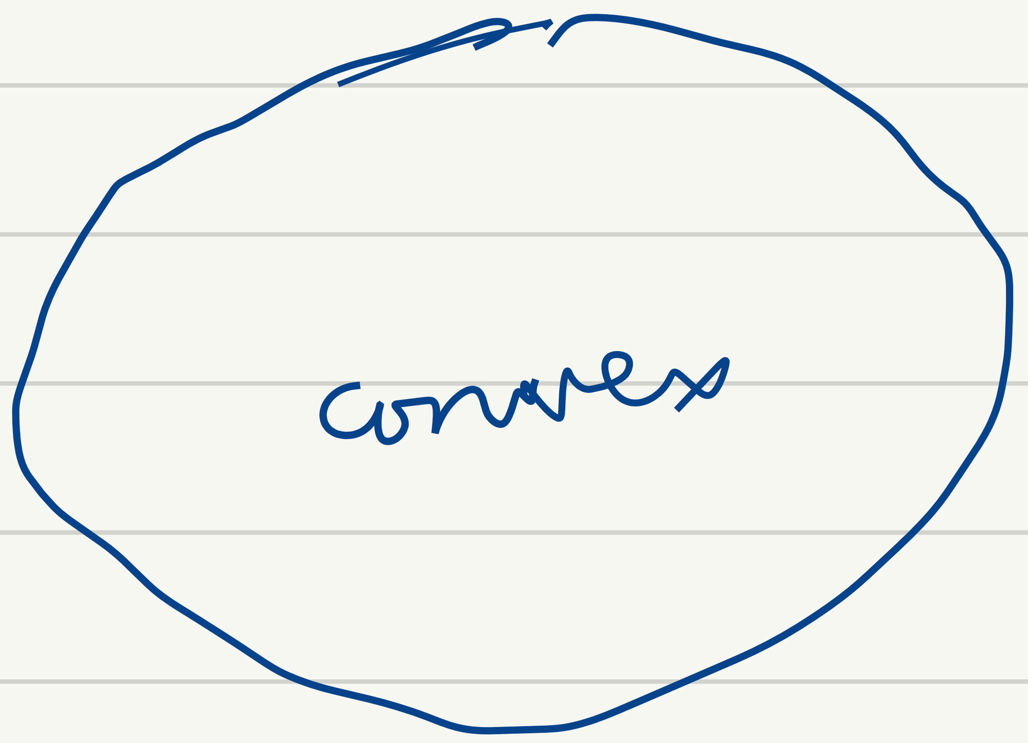
Continuous opt.

- uncon. ✓
- con. ✗
- Convex ✓
- nonconvex ?

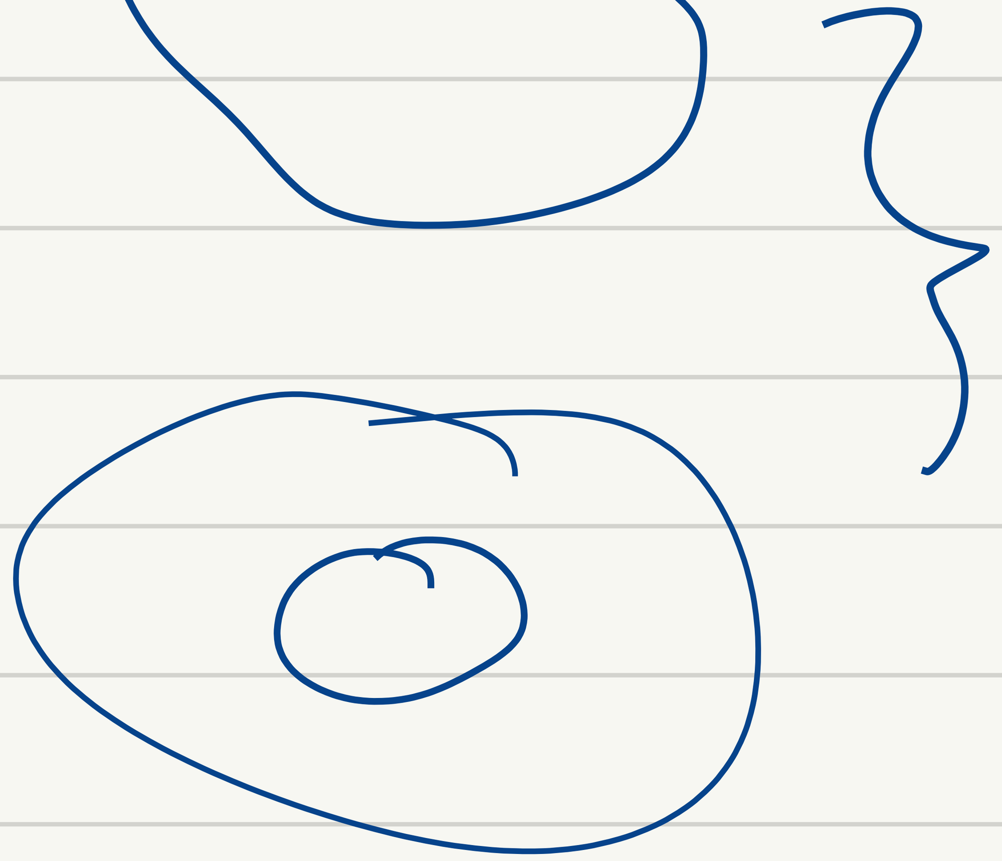
S is convex set

f is convex function

Convex set

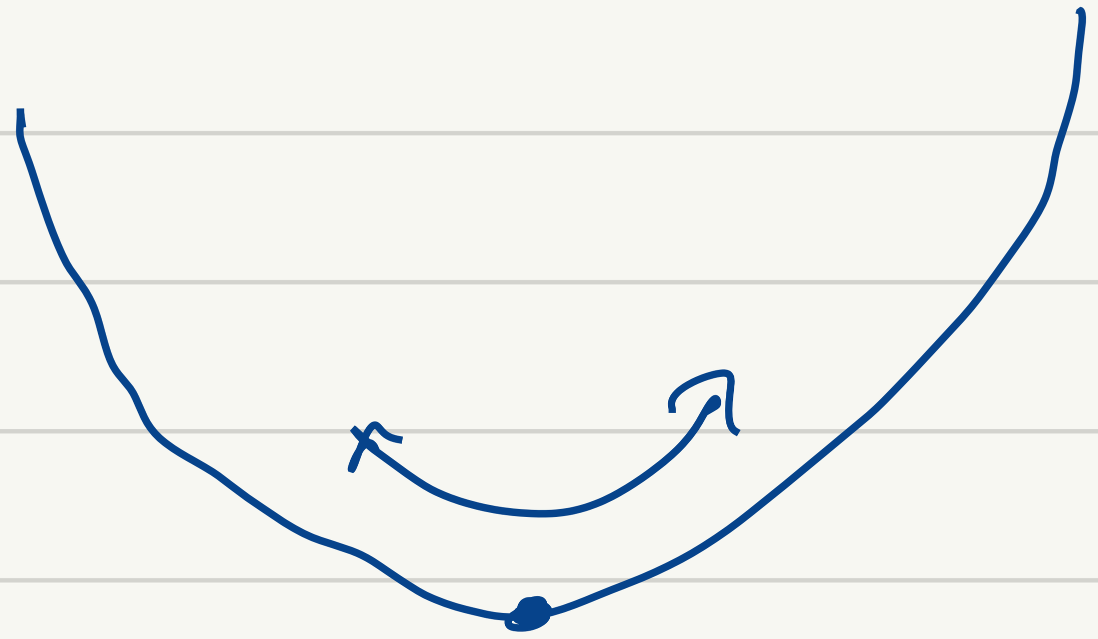


not convex

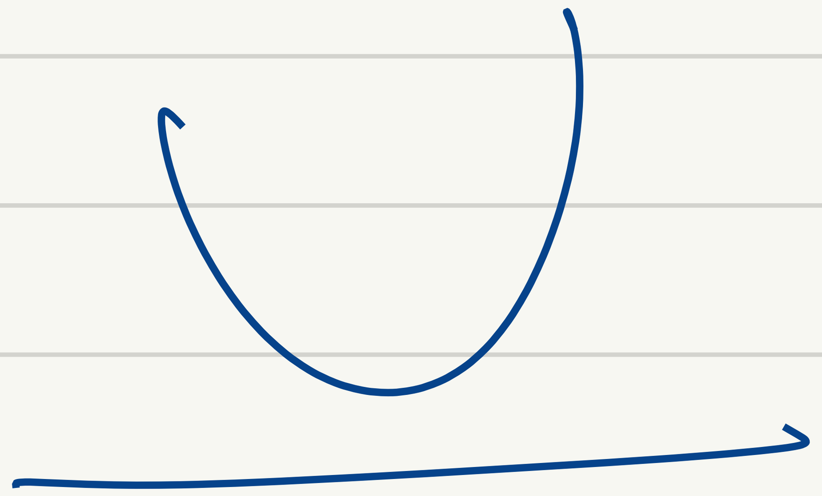


Convex function

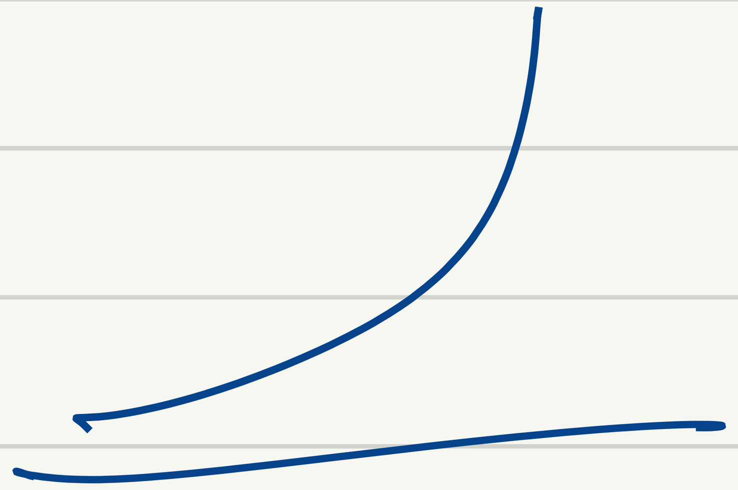
non convex



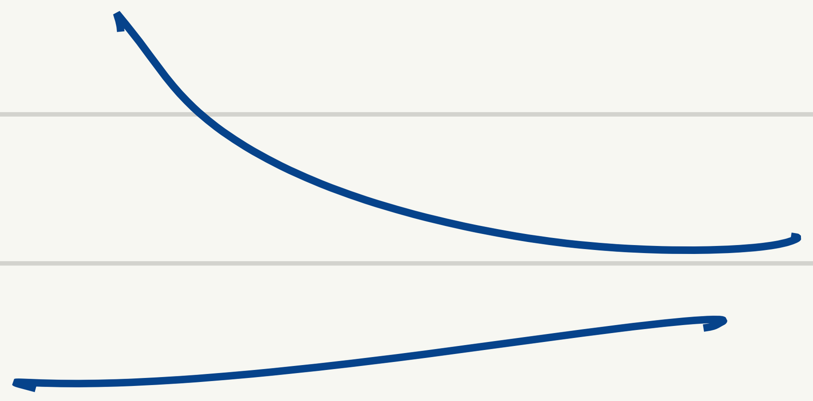
convex



x^2



e^x



e^{-x}