Session 9: Convex functions

Optimization and Computational Linear Algebra for Data Science

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Optimization

In machine learning, we often have to minimize functions

$$f(\theta) = \mathrm{Loss}(\mathrm{data}, \mathrm{model}_\theta) \quad \text{with respect to} \quad \underbrace{\theta \in \mathbb{R}^n}_{\text{model's parameters}}.$$

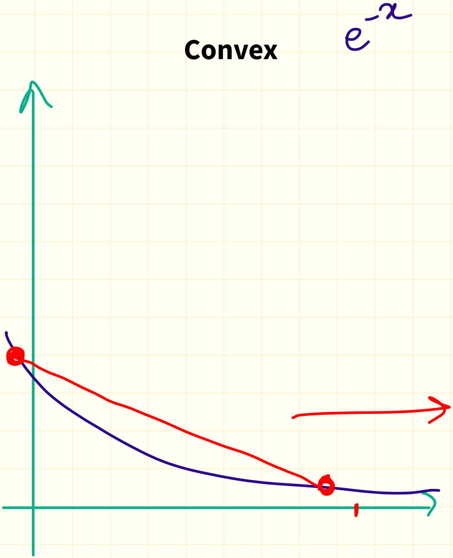
- For $n = 1, 2$, one could plot f to find the minimizer.
- This is intractable for larger dimension.

We will

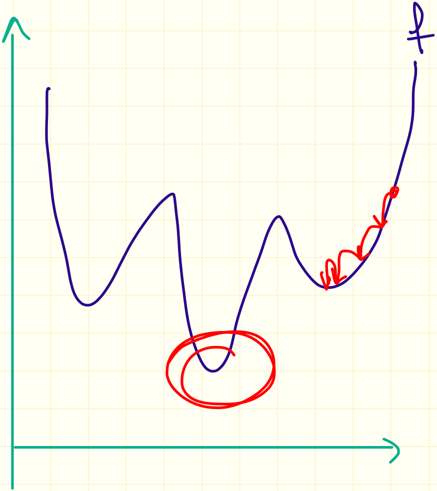
- focus on convex cost functions f.
- study gradient descent algorithms to minimize f.

Convex vs non-convex

Convex



Non-convex

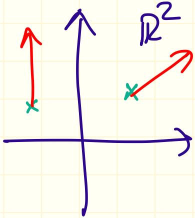


Gradient/Hessian

For $f : \mathbb{R}^n \to \mathbb{R}$:

- Gradient at $x \in \mathbb{R}^n$:

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{pmatrix} \in \mathbb{R}^n$$



- Hessian at $x \in \mathbb{R}^n$:

$$H_f(x) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2}(x) & \frac{\partial^2 f}{\partial x_1\,\partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n}(x) \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1}(x) & \frac{\partial^2 f}{\partial x_2^2}(x) & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1}(x) & \frac{\partial^2 f}{\partial x_n\,\partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(x) \end{pmatrix} \in \mathbb{R}^{n\times n}$$

Taylor's formulas

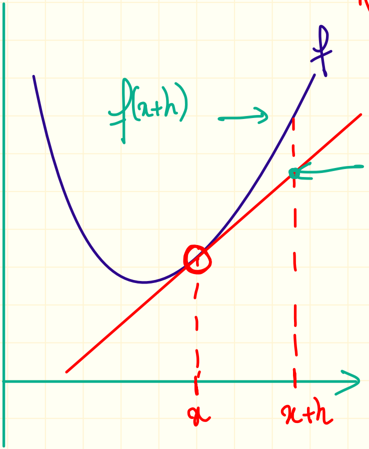
Let $x \in \mathbb{R}^n$. Heuristically, for $h \in \mathbb{R}^n$ "small", we have

$$f(x+h) \simeq f(x) + \langle \nabla f(x), h \rangle.$$

$u \cdot v$

$\langle u, v \rangle$ = dot product between u and v

not mathematically correct



$f(x) + \langle \nabla f(x), h \rangle$

"Rigorous Taylor"

$$\boxed{f(x+h) = f(x) + \nabla f(x) \cdot h + Err_1(h)}$$

$$\boxed{\frac{Err_1(h)}{\|h\|} \xrightarrow[h \to 0]{} 0}$$

0,001

Taylor's formulas

Let $x \in \mathbb{R}^n$. Heuristically, for $h \in \mathbb{R}^n$ "small", we have

$$f(x+h) \simeq f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2} h^\top H_f(x) h.$$

$$+ \ \mathrm{Err}_2(h)$$

$$\frac{\mathrm{Err}_2(h)}{\|h\|^2} \xrightarrow[h \to 0]{} 0$$

h^2

$$f : \mathbb{R} \to \mathbb{R}, \quad f(x+h) \simeq f(x) + f'(x)h + \frac{1}{2} h f''(x) h$$

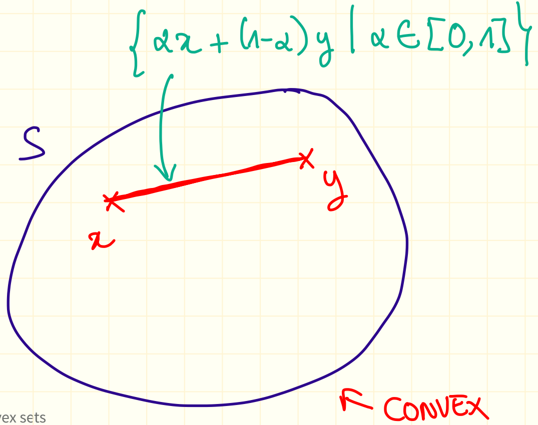
Convex sets

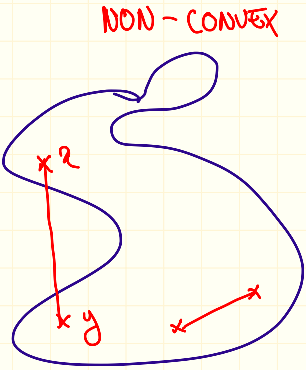
Convex set

Definition

A set $S \subset \mathbb{R}^n$ is called a convex set if for all $x, y \in S$ and all $\alpha \in [0, 1]$,

$$\alpha x + (1 - \alpha) y \in S.$$





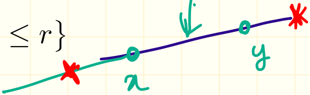
Exercise

1. Show that any subspace S of $\mathbb{R}^n$ is convex.
2. Let $\|\cdot\|$ be a (arbitrary) norm and $r \geq 0$. Show that the "ball" of radius r:

$$B(r) = \{x \in \mathbb{R}^n \mid \|x\| \leq r\}$$

is convex.

$\alpha x + (1-\alpha) y$



① Let $x, y \in S$ and $\alpha \in [0,1]$, since S is closed under linear combinations, $\alpha x + (1-\alpha) y \in S$, S is convex

② Let $x, y \in B(r)$, $\alpha \in [0,1]$

$$\|\alpha x + (1-\alpha) y\| \leq \|\alpha x\| + \|(1-\alpha) y\| = \alpha \|x\| + (1-\alpha)\|y\|$$

triangular ineq.

$$\leq \alpha r + (1-\alpha) r = r$$

$\longrightarrow \alpha x + (1-\alpha) y \in B(r)$.

Convex functions

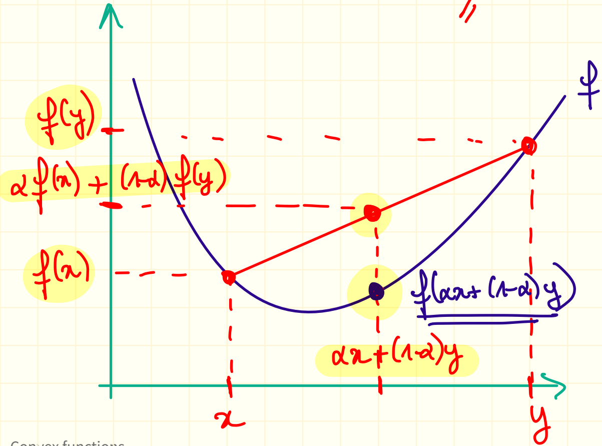
Convex / concave functions

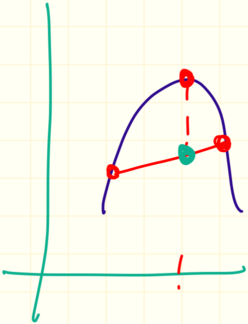
Definition

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for all $x, y \in \mathbb{R}^n$ and all $\alpha \in [0, 1]$,

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y). \tag{1}$$

$\geq$





Convex / concave functions

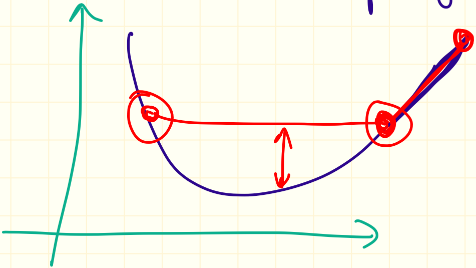
Definition

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for all $x, y \in \mathbb{R}^n$ and all $\alpha \in [0,1]$,

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y). \tag{1}$$

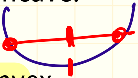
- We say that f is *strictly convex* is there is strict inequality in (1) whenever $x \neq y$ and $\alpha \in (0,1)$.
- A function f is called concave if $-f$ is convex.

$\longrightarrow$ inequality in the other direction.



Exercise

1. Show that any linear map $f : \mathbb{R}^n \to \mathbb{R}$ is convex and concave.
2. Show that a norm $\| \cdot \|$ is convex.
3. Show that the sum of two convex functions is also a convex function.



$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y)$$

① Let $x, y \in \mathbb{R}^n$ and $\alpha \in [0,1]$

$$f(\alpha x + (1-\alpha) y) \overset{①}{\leq} \alpha f(x) + (1-\alpha) f(y)$$
$$\overset{}{=}$$
$$\overset{②}{\geq}$$

because f is linear

① → f is convex   ② → f is concave

② $\|\alpha x + (1-\alpha) y\| \leq \|\alpha x\| + \|(1-\alpha) y\| = \underbrace{\alpha}_{\geq 0} \|x\| + \underbrace{(1-\alpha)}_{\geq 0} \|y\|$

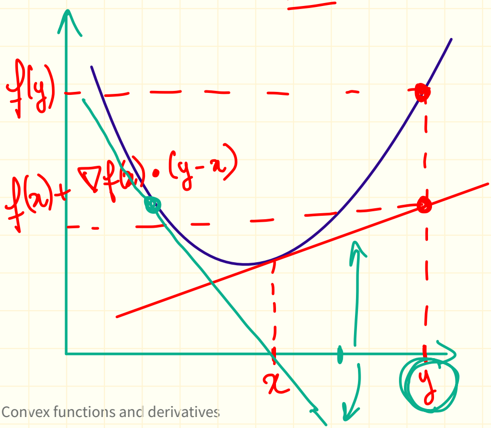
by trig. inequality.

Convex functions and derivatives

Proposition

A differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if and only if for all $x, y \in \mathbb{R}^n$

$$f(\underbrace{y}_{x+h}) \geq f(x) + \langle \nabla f(x), \underbrace{(y - x)}_{h} \rangle.$$

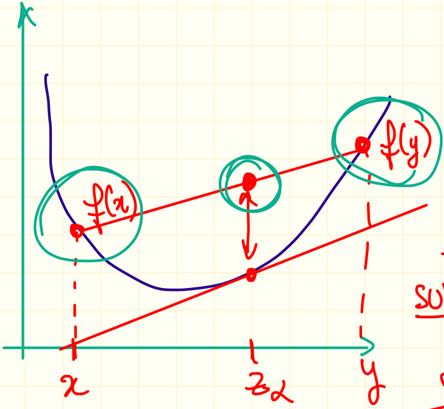


" The graph of a convex function is above its tangents "

Proof

$\Leftarrow$ Let's assume that for all $x, y \in \mathbb{R}^n$, $f(y) \geq f(x) + \nabla f(x) \cdot (y - x)$

Let $x, y \in \mathbb{R}^n$ and $\alpha \in [0,1]$, define $z_\alpha = \alpha x + (1-\alpha) y$.



Applying the inequality twice:

$$\alpha f(x) \geq \alpha f(z_\alpha) + \nabla f(z_\alpha) \cdot (\alpha x - \alpha z_\alpha)$$

$$(1-\alpha) f(y) \geq (1-\alpha) f(z_\alpha) + \nabla f(z_\alpha) \cdot ((1-\alpha) y - (1-\alpha) z_\alpha)$$

SUM: $\alpha f(x) + (1-\alpha) f(y)$

$$\geq f(z_\alpha) + \cancel{\nabla f(z_\alpha) \cdot \underbrace{\left(\alpha x + (1-\alpha) y - z_\alpha\right)}_{=0}}$$

$\rightarrow$ f is convex

Proof

$\Rightarrow$) Let assume that f is convex.

Let $x, y \in \mathbb{R}^n$, let $t \in [0,1]$. write $\boxed{z_t = (1-t)x + ty}$.

$= x + t(y-x)$

Taylor's formula: $f(z_t) = f(x + \overbrace{t(y-x)}^{h})$

$= f(x) + t\nabla f(x)\cdot(y-x) + Err_1(t)$

f is convex $\quad f(z_t) \leqslant (1-t)f(x) + tf(y)$

Combining: $\quad tf(y) \geqslant tf(x) + t\nabla f(x)\cdot(y-x) + Err_1(t)$

$$\boxed{f(y) \geqslant f(x) + \nabla f(x)\cdot(y-x)} + \frac{Err_1(t)}{t}$$

$\xrightarrow{t \to 0} 0$

Proof

Minimizers of a convex function

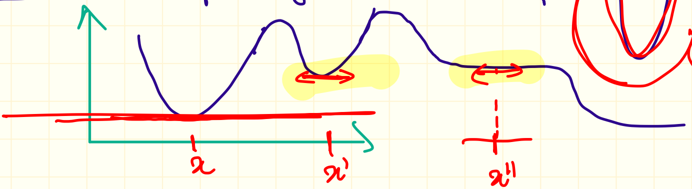
$$f(x+h) \simeq f(x) + \underbrace{\cancel{\nabla f(x)}}_{=0} \cdot h + \frac{1}{2} h^T Hf(x) h$$

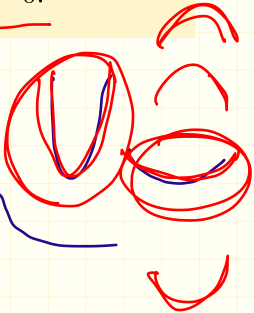
Corollary

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable $\boxed{\text{convex}}$ function and $x \in \mathbb{R}^n$.
Then

$$x \text{ is a minimizer of } f \iff \nabla f(x) = 0.$$

Proof: $\Rightarrow$) True for any differentiable f





$\Leftarrow$) Let $y \in \mathbb{R}^n$, $f(y) \geq f(x) + \underbrace{\nabla f(x)}_{=0} \cdot (y - x)$

$\geq f(x) \rightarrow x$ is a minimizer of f.

Hessian of convex function

Proposition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice-differentiable function. Then f is convex if and only if for all $x \in \mathbb{R}^n$, $H_f(x)$ is positive semi-definite.

Recall :
- a matrix M is PSD if for all $v \in \mathbb{R}^n$, $v^T M v \geq 0$
- this is equivalent to saying that all the eigenvalues of M are ≥ 0

Example : $f(x) = \|x\|^2 = x_1^2 + \dots + x_n^2$

For all $x \in \mathbb{R}^n$, $H_f(x) = 2 I_{d_n} \leftarrow$ PSD hence f is convex

Hessian of convex function

Proposition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice-differentiable function. Then f is convex if and only if for all $x \in \mathbb{R}^n$, $H_f(x)$ is positive semi-definite.

Remark: if $f : \mathbb{R} \to \mathbb{R}$ is twice differentiable:

f is convex $\iff$ $f''(x) \geq 0$ for all $x \in \mathbb{R}$

Remark: If $H_f(x)$ is Positive definite for all $x \in \mathbb{R}^n$ then f is strictly convex. But the converse is not true in general.

Proof idea: $f(y) \underset{\geq}{\simeq} f(x) + \nabla f(x) \cdot (y-x) + \underbrace{\frac{(y-x)^T H_f(x) (y-x)}{2}}_{\geq 0}$

Jensen’s inequality

Jensen's inequality

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a convex function. Then for all $x_1, \ldots, x_k \in \mathbb{R}^n$ and all $\alpha_1, \ldots, \alpha_k \geq 0$ such that $\sum_{i=1}^k \alpha_i = 1$ we have

concave

f("average") $\longrightarrow$

$$f\left(\sum_{i=1}^k \alpha_i x_i\right) \leq \sum_{i=1}^k \alpha_i f(x_i).$$

$\leftarrow$ "average of the f's"

$\geq$ $\leftarrow$ if f is concave

More generally, if X is a random variable that takes value in $\mathbb{R}^n$ we have

$$\boxed{f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)].}$$

$\geq$

Example • $f: \mathbb{R} \to \mathbb{R}$, $x \mapsto x^2$ is convex therefore,

for any random variable X, $\mathbb{E}[X]^2 \leq \mathbb{E}[X^2]$

$Var(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2 \geq 0$

Example: entropy

- Let's consider a random variable X taking values in $\{1, \dots k\}$
- Let's write $p_i = \mathbb{P}(X = i)$ for $i \in \{1, \dots k\}$.

The entropy of X is defined as:

$$\boxed{H(X) = \sum_{i=1}^{k} p_i \log\Big(\underbrace{\frac{1}{p_i}}_{\geq 0}\Big)} \geq 0$$

log is a concave function (exercise!) hence, by Jensen:

$$H(X) = \sum_{i=1}^{k} \underbrace{p_i}_{\text{"}\alpha_i\text{"}} \overbrace{\log}^{g}\Big(\overbrace{\frac{1}{p_i}}^{\text{"}x_i\text{"}}\Big) \leq \overbrace{\log}^{g}\Big(\sum_{i=1}^{k} \underbrace{p_i}_{\text{"}\alpha_i\text{"}} \cdot \overbrace{\frac{1}{p_i}}^{\text{"}x_i\text{"}}\Big) = \log(k)$$

Example: entropy

$\longrightarrow 0 \leq H(X) \leq \log(k)$

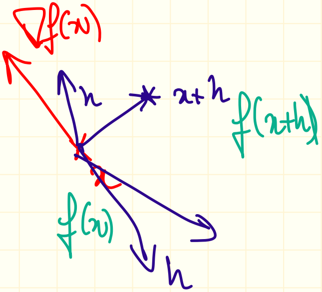
The value $\log(k)$ is achieved for $p_i = \frac{1}{k}$ for all i:

$$H(X) = \sum_{i=1}^{k} \frac{1}{k} \log\left(\frac{1}{\frac{1}{k}}\right) = \log(k)$$

The entropy is maximal when X is uniformly distributed over $\{1, \ldots k\}$

Questions?

$$f(x+h) \simeq f(x) + \langle h, \nabla f(x) \rangle$$



$$\max \{ \underline{v \cdot x} \mid \|v\| = 1 \}$$

Questions?

$$\#\text{paths}(k+1, i \to j) = \sum_{\ell \text{ neighbor of } j} \#\text{paths}(k, i \to \ell)$$

$$\frac{\nabla f(x)}{\|\nabla f(x)\|} = \underset{\substack{v \in \mathbb{R}^n \\ \|v\|=1}}{\operatorname{argmax}} \lim_{\substack{t \to 0 \\ >}} \boxed{\frac{f(x+tv) - f(x)}{t}}$$