

Master-MIRI

Topics on Optimization and Machine Learning (TOML)

José M. Barceló Ordinas
Departament d'Arquitectura de Computadors
(UPC)

Topic 1: Convex Optimization Problems. Convex Functions.

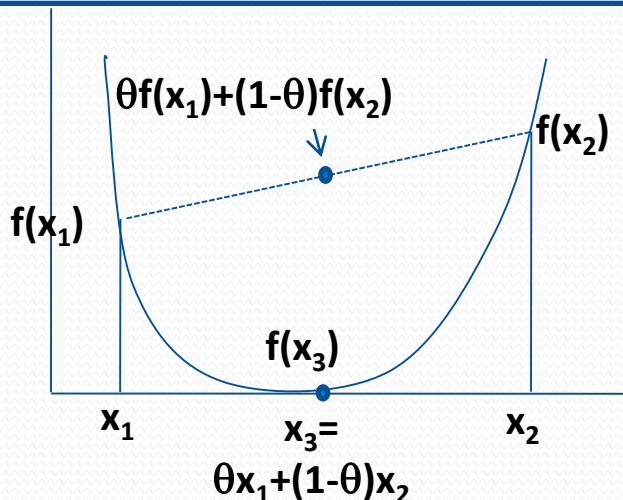
• Domains of a function and Convex Functions

A function $f: A \longrightarrow B$ is a **mapping** between sets A and B . The **domain** of a function is the “input” parameters of the function, it is to say, all $x \in \text{dom } f \subset A$ if $f(x) \subset B$ exists.

A function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ is **convex** if

- For all $x \in \text{dom } f \subset \mathbb{R}^n$, then $\text{dom } f$ is a convex set
- For $0 \leq \theta \leq 1$, we have $f(\theta x_1 + (1-\theta)x_2) \leq \theta f(x_1) + (1-\theta)f(x_2)$

- Strict convexity \rightarrow change “ \leq ” for “ $<$ ”
- A function “ f ” is concave if “ $-f$ ” is convex
- Affine functions, $f(x) = Ax + b$ (and therefore also linear functions, $f(x) = Ax$), hold equality in condition ii) and thus are both convex and concave



- Linear functions and affine functions

In **analytic geometry**, a linear function is a polynomial: e.g. in one dimension $f(x) = ax+b$ or in more dimensions $f(x_1, \dots, x_n) = a_1 x_1 + \dots + a_n x_n$ is a hyperplane.

In **linear algebra**, a linear function (or linear map) is a mapping between 2 vector spaces that preserves addition and scalar multiplication: $f(\alpha x + \beta y) = \alpha f(x) + \beta f(y)$, where x, y are vectors

An **affine function** is the composition of a translation and a linear map. For example, if A is a matrix, $f(x) = Ax$ is a linear function (linear map) and affine and $f(x) = Ax+b$ is an affine function (but not linear).

Topic 1: Convex Optimization Problems. Convex Functions.

• Reminder

- Let $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ a function

The function f is **differentiable** if $\text{dom } f$ is open and there exists the partial derivative (is a vector) at each point $x \in \text{dom } f \subset \mathbb{R}^n$

$$\nabla f(x) = (\delta f(x)/\delta x_1, \delta f(x)/\delta x_2, \dots, \delta f(x)/\delta x_n)$$

The function is twice differentiable if the $\text{dom } f$ is open and the **Hessian** $\nabla^2 f$ (is a matrix) exists at each point $x \in \text{dom } f \subset \mathbb{R}^n$

$$\nabla^2 f(x)_{ij} = \delta^2 f(x) / \delta x_i \delta x_j$$

A matrix A is **positive semi-definite** iff $\forall x, x^T A x \geq 0$ (**positive definite** if $x^T A x > 0$). Ways of checking whether a matrix is positive semi-definite/definite is:

- All eigenvalues of A are ≥ 0 (positive definite \rightarrow all are > 0)
- All leading principal minors have positive or equal to zero determinants (positive definite \rightarrow all are > 0)

A matrix A is **negative semi-definite** iff $\forall x, x^T A x \leq 0$ (**negative definite** if $x^T A x < 0$). Ways of checking whether a matrix is negative semi-definite/definite is:

- All eigenvalues of A are ≤ 0 (negative definite \rightarrow all are < 0)
- All leading **odd** principal minors have **negative** or equal to zero determinants and all **even** principal minors have **positive** or equal to zero determinants (negative definite \rightarrow odd are < 0 and even are > 0)

- **Reminder**

Critical point of a function of a real variable is any value in the domain where either the function is not differentiable or its derivative is 0.

If the derivative is zero, the point is called a **stationary point** of the function. Then a stationary point is a critical point but not all critical points are stationary (e.g. there is no derivative).

An **inflection point** (is a stationary point) is a point on a curve at which the curvature or concavity changes sign from plus to minus or from minus to plus, i.e., a point on a curve at which the second derivative changes sign and the first derivative is 0.

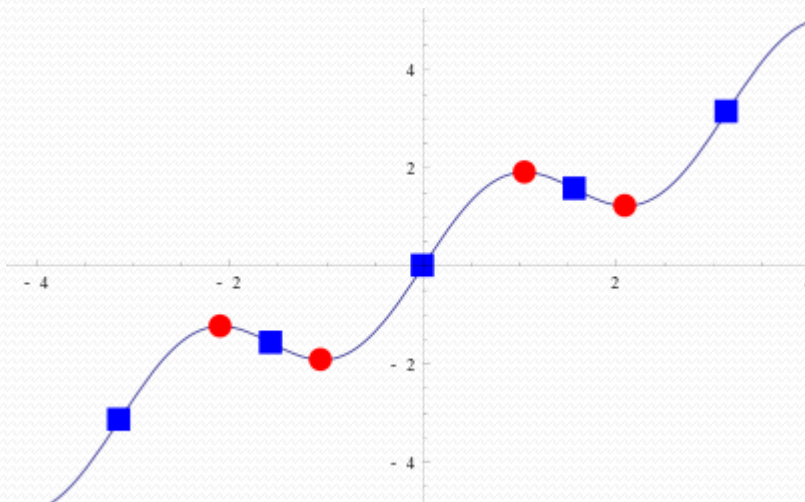
Local maxima and minima of a function can occur only at its critical points. But, not every stationary point is a maximum or a minimum of the function, e.g. not at inflection points.

Topic 1: Convex Optimization Problems. Convex Functions.

• Reminder

If the second derivative is positive is a minimum (stationary point) and if it is negative it is a maximum (stationary point).

If the second derivative is zero, the nature of the stationary point must be determined by way of other means, often by noting a sign change around that point provided the function values exist around that point.



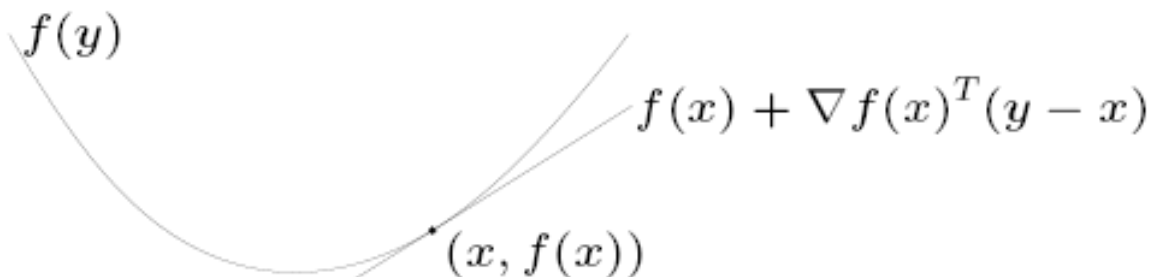
Blue squares: inflection points
Red dots: maximum or minimum

• First-order conditions

Let $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ be differentiable, it is to say ∇f exists in the whole domain of f . Then f is convex iif

- i. **dom f** is a convex set,
- ii. **$f(y) \geq f(x) + \nabla f(x)^T(y - x)$** (first order Taylor approximation of f near x) for all $x, y \in \text{dom } f$

From **local information** about a convex function, a **global information** is obtained.



first-order approximation of f is global underestimator

• Second-order conditions

Let $f: \mathbb{R}^n \rightarrow \mathbb{R}$ be twice differentiable, it is to say the Hessian $\nabla^2 f$ exists in the whole domain of f . Then f is convex iff

- i. **dom f** is a convex set,
- ii. **$H = \nabla^2 f(x) \geq 0$** , the Hessian matrix is positive semi-definite.

Be careful, condition i) is necessary: $f(x) = 1/x^2$ in $\text{dom } f = \{x \in \mathbb{R}, x \neq 0\}$ has $f''(x) > 0$ for all $x \in \text{dom } f$, but is not convex.

• Examples:

- All **affine and linear functions** are convex, and concave functions,
- **Quadratic functions:** $f(x) = \frac{1}{2}x^T P x + q^T x + r$ are convex for all $P \geq 0$ (positive semi-definite) matrices and $x \in \mathbb{R}^n$,
- **Exponential functions:** e^{ax} is convex on \mathbb{R} and any $a \in \mathbb{R}$,

- **More examples:**

- **Powers of absolute value** $|x|^a$ with $a \geq 1$ are convex on \mathbb{R} ,
- **Logarithms** $\log x$ is concave on \mathbb{R}_{++} ,
- **Negative entropy** $x \log x$ is convex on \mathbb{R}_+ ($0 \log 0 = 0$),
- Any **norm** $\|\cdot\|_p$ is convex on \mathbb{R}^n ,
- **Max function**, $f(x) = \max\{x_1, x_2, \dots, x_n\}$ is convex on \mathbb{R}^n ,
- **Quadratic over linear function** $f(x, y) = x^2/y$ is convex on $\mathbb{R} \times \mathbb{R}_{++}$,
- **Log-sum-exp**, $f(x) = \log(e^{x_1} + e^{x_2} + \dots + e^{x_n})$ is convex on \mathbb{R}^n ,
- **Geometric mean** $f(x) = (\prod_{i=1}^n x_i)^{1/n}$ is concave on \mathbb{R}_{++}^n ,
- **Log-determinant**, $f(x) = \log(\det A)$ is concave on S^n_{++} where S^n_{++} is the set of symmetric positive definite $n \times n$ matrices.

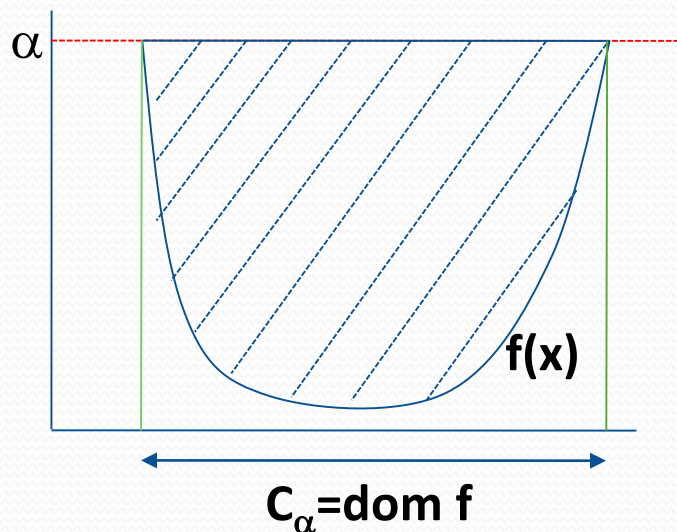
• Sub-level sets

A **α -sublevel** set of a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as

$$C_\alpha = \{x \in \text{dom } f \mid f(x) \leq \alpha\}$$

Where we define **α -level** sets when equality. **Sublevel sets** of a convex function **are convex** for any α (converse is false: convexity of a sublevel does not imply convexity in the function).

If f is concave, **α -superlevel** sets are defined as $C_\alpha = \{x \in \text{dom } f \mid f(x) \geq \alpha\}$ and are convex.



Proof:

If $x_1, x_2 \in C_\alpha$, then $f(x_1) \leq \alpha$, $f(x_2) \leq \alpha$

Then:

$$\begin{aligned} f(\theta x_1 + (1-\theta)x_2) &\leq \theta f(x_1) + (1-\theta)f(x_2) \leq \\ &\leq \theta\alpha + (1-\theta)\alpha \leq \alpha \quad \text{for } 0 \leq \theta \leq 1 \end{aligned}$$

Then $\theta x_1 + (1-\theta)x_2 \in C_\alpha$

- **α -level set of a quadratic function:**

- $f(x) = \frac{1}{2}x^T P x$ with P positive definite matrix. Then:

$$C_{\alpha}^{-} = \{x \in \text{dom } f \mid \frac{1}{2}x^T P x = \alpha\}$$

Is an ellipsoid with center 0.

- Proof:

$$f(x) = \frac{1}{2}x^T P x + q^T x = \frac{1}{2}(x + P^{-1}q)^T P (x + P^{-1}q) - \frac{1}{2}q^T P^{-1}q$$

Then, the level set $C_{\alpha}^{-} = \{x \in \text{dom } f \mid f(x) = \alpha\}$ forms an ellipsoid of center $x_0 = -P^{-1}q$

Remember the equation of an ellipsoid:

$$E = \{x \mid \frac{1}{2}(x - x_0)^T P (x - x_0) = \alpha\}$$

Topic 1: Convex Optimization Problems. Convex Functions.

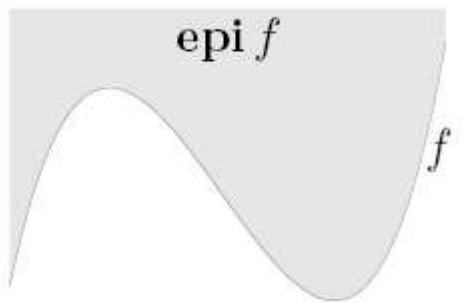
• Epigraphs/Hypographs

The graph of a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as

$$\{(x, f(x)) \mid x \in \text{dom } f\}$$

The **epigraph** of a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as

$$\text{epi } f = \{(x, t) \mid x \in \text{dom } f \text{ and } f(x) \leq t\} \subset \mathbb{R}^{n+1}$$



The **hypograph** of a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is defined as

$$\{(x, t) \mid x \in \text{dom } f \text{ and } f(x) \geq t\} \subset \mathbb{R}^{n+1}$$

A function is **convex** iff its epigraph is a **convex set**

A function is **concave** iff its hypograph is a **convex set**

The epigraph definition gives another tool to test whether a function is convex or not

- **Jensen inequality**

The inequality $f(\theta x_1 + (1-\theta)x_2) \leq \theta f(x_1) + (1-\theta)f(x_2)$ also is called **Jensen inequality** and can be extended to k points, if f convex and $x_1, x_2, \dots, x_k \in \text{dom } f$ and $\theta_1 + \theta_2 + \dots + \theta_k = 1$, then

$$f(\theta_1 x_1 + \theta_2 x_2 + \dots + \theta_k x_k) \leq \theta_1 f(x_1) + \theta_2 f(x_2) + \dots + \theta_k f(x_k)$$

and as in the case of convex sets, this inequality extends to infinite sums, integrals and expectations, e.g.:

- $f(\int_S p(x) x \, dx) \leq \int_S f(x) p(x) \, dx$ if the integral exists
- $f(E(x)) \leq E(f(x))$ where $E(\cdot)$ is the expectation of r.v. x

Topic 1: Convex Optimization Problems. Convex Functions.

• Conjugate Function

The function $f^*: \mathbb{R}^n \rightarrow \mathbb{R}$ is called the **conjugate function**, with f^* defined as:

$$f^*(y) = \sup_x (\langle x, y \rangle - f(x)) = \sup_x (y^T x - f(x))$$

The conjugate function is convex

- It can be interpreted as the negative of the y-intercept of the tangent line to the graph of f that has slope y . In other words, we look for the largest affine function below f , it is to say, the one with largest intercept.
- It can also be interpreted as an encoding of the convex hull of the function's epigraph in terms of its supporting hyperplanes.

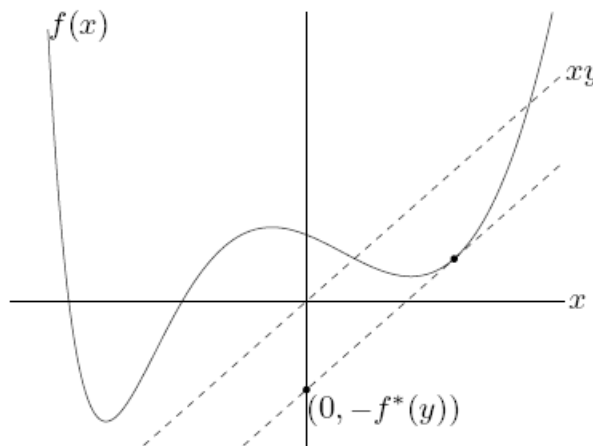


Figure 3.8 A function $f : \mathbb{R} \rightarrow \mathbb{R}$, and a value $y \in \mathbb{R}$. The conjugate function $f^*(y)$ is the maximum gap between the linear function yx and $f(x)$, as shown by the dashed line in the figure. If f is differentiable, this occurs at a point x where $f'(x) = y$.

Topic 1: Convex Optimization Problems. Convex Functions.

It can also be interpreted as an encoding of the convex hull of the function's epigraph in terms of its supporting hyperplanes.

$$f^*(y) = \sup_x (\langle x, y \rangle - f(x)) = \sup_x (y^T x - f(x))$$

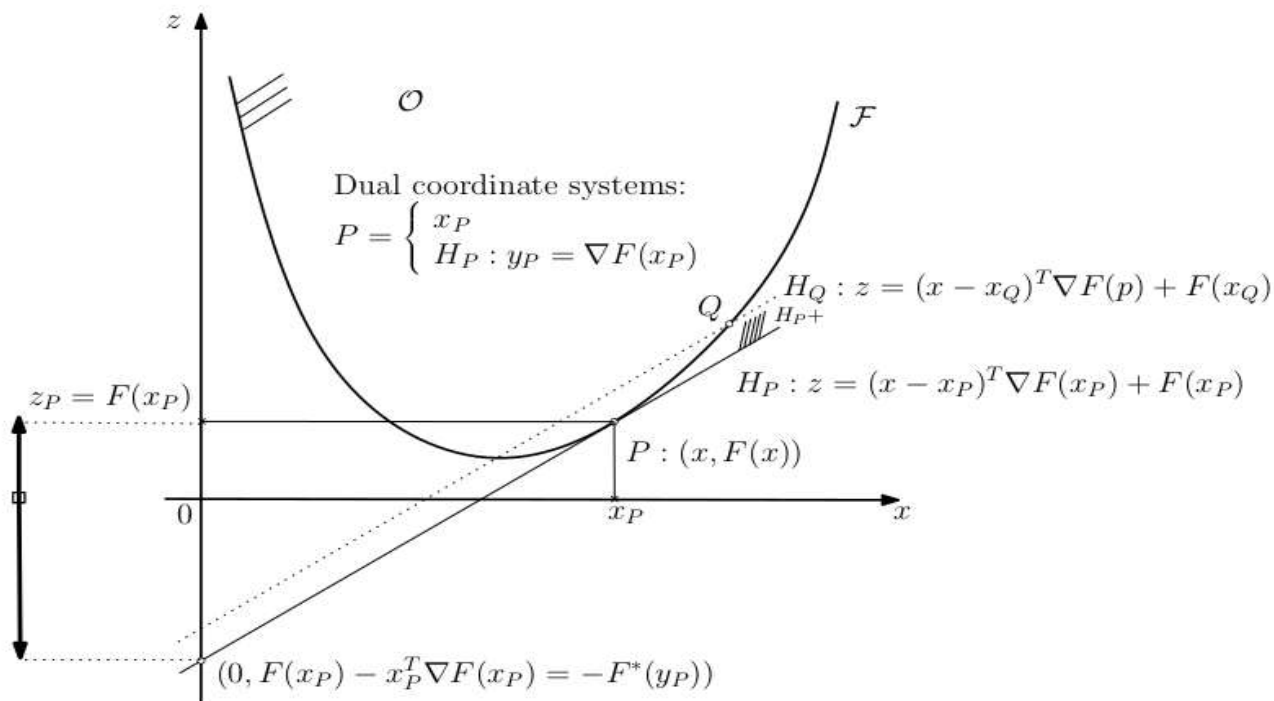


Figure 1: Illustration the Legendre transformation of a strictly convex function: A point P on the boundary of \mathcal{O} can either be parameterized by using the x -coordinate system, or by using the dual slope $y = \nabla F(x)$ coordinate system. For a point $P \in \partial \mathcal{O}$ with x -coordinate x_P , and tangent parameter $y_P = \nabla F(x_P)$, the Legendre conjugate $F^*(y)$ reads as the intersection of the hyperplane H_P with the the z -axis. The object \mathcal{O} is either interpreted as the convex hull of the points, or dually as the intersection of the supporting half-spaces.

• Conjugate Function

The function $f^*: \mathbb{R}^n \rightarrow \mathbb{R}$ is called the **conjugate function**, with f^* defined as:

$$f^*(y) = \sup_x (\langle x, y \rangle - f(x)) = \sup_x (y^T x - f(x))$$

The conjugate function is convex

It can be interpreted as the negative of the y -intercept of the tangent line to the graph of f that has slope y . In other words, we look for the largest affine function below f , it is to say, the one with largest intercept.

- If f is convex and differentiable \rightarrow **Legendre transform**: the x value that attains the maximum satisfies that $y = \nabla_x f(x)$ and then:

$$f^*(y) = \sup_x (y^T x - f(x)) = (x^T \nabla_x f(x) - f(x)) = f^*(\nabla_x f(x))$$

- $f^{**} = f$ iff f is convex and closed (i.e. $\text{epi } f$ is closed)

- **Conjugate Function**

- **Examples:**

- **Affine function:** $f(x)=ax+b \rightarrow f^*(y)=-b$ at $y=a$
 - **Exponential:** $f(x)=e^x \rightarrow f^*(y)=y \log(y) - y$ with $\text{dom } f^* = \mathbb{R}_+$
 - **Negative entropy:** $f(x)=x \log(x) \rightarrow f^*(y)=e^{y-1}$ with $\text{dom } f^* = \mathbb{R}$
 - **Indicator function:** $f_S(x)=0$ if $x \in S \rightarrow f^*(y) = \sup_x (y^T x)$
 - **Log-sum-exp:** $f(x)=\log(\sum_{i=1..m} \exp(x_i)) \rightarrow f^*(y) = \sum_{i=1..m} y_i \log(y_i)$ with $1^T y = 1$ and $y \geq 0$

• Operations that preserve convexity

- **Non-negative weighted sums:** $f = w_1 f_1 + \dots + w_m f_m$ is convex if f_i is convex and $w_i \geq 0$ for $i = 1, \dots, m$
- **Non-negative weighted integrals:** $g(x) = \int_A w(y) f(x, y) dy$ is convex if $f(x, y)$ is convex in x and $w(y) \geq 0$ for each $y \in A$
- **Composition with an affine mapping:** $f: \mathbb{R}^n \longrightarrow \mathbb{R}$, $A \in \mathbb{R}^{n \times m}$, $b \in \mathbb{R}^n$, and let be $g: \mathbb{R}^m \longrightarrow \mathbb{R}$ such as $g(x) = f(Ax + b)$ with $\text{dom } g = \{x \mid Ax + b \in \text{dom } f\}$. Then, if f is convex (concave), so is g .
- **Pointwise maximum:** $g(x) = \max\{f_1(x), \dots, f_m(x)\}$ is convex if f_i is convex for $i = 1, \dots, m$
- **Pointwise supremum:** $g(x) = \sup_{y \in A} \{f(x, y)\}$ is convex if $f(x, y)$ is convex in x for each $y \in A$. The domain of g is, $\text{dom } g = \{x \mid (x, y) \in \text{dom } f \text{ for all } y \in A, \sup_{y \in A} \{f(x, y)\} < \infty\}$.

• Composition

- Let be $h: \mathbb{R}^k \longrightarrow \mathbb{R}$ and $g: \mathbb{R}^n \longrightarrow \mathbb{R}^k$ functions, and let us consider composition $f=h \circ g=h(g(x)): \mathbb{R}^n \longrightarrow \mathbb{R}^k \longrightarrow \mathbb{R}$, with $\text{dom } f=\{x \in \text{dom } g \mid g(x) \in \text{dom } h\}$.
- Let us consider the cases, $k=1$ and $n=1$, $h: \mathbb{R} \longrightarrow \mathbb{R}$, $g: \mathbb{R} \longrightarrow \mathbb{R}$ and remember that $f'(x)=h'(g(x)) g'(x)$ and that $f''(x)=h'(g(x)) (g'(x))^2 + h'(g(x)) g''(x)$. In order to be convex, $f''(x) \geq 0$

f is convex if h is convex and non-decreasing and g is convex
f is convex if h is convex and non-increasing and g is concave
f is concave if h is concave and non-decreasing and g is concave
f is concave if h is concave and non-increasing and g is convex

- Similar conditions for $n > 1$, but with considering the extended-value function of h which assigns values to $\pm\infty$

• Examples of Composition

- If g is convex $\rightarrow f(\mathbf{x})=e^{g(\mathbf{x})}$ is convex
- If g is concave and positive $\rightarrow \log(g(\mathbf{x}))$ is concave
- If g is concave and positive $\rightarrow 1/g(\mathbf{x})$ is convex
- If g is convex and non-negative and $p \geq 1 \rightarrow g(\mathbf{x})^p$ is convex
- If g is convex $\rightarrow -\log(-(g(\mathbf{x})))$ is convex on $\{\mathbf{x} | g(\mathbf{x}) < 0\}$

• Vector Composition

- Let us now consider $h:\mathbb{R}^k \longrightarrow \mathbb{R}$ and $g_i:\mathbb{R}^n \longrightarrow \mathbb{R}$ functions, and let us consider composition $f=h(g_1(x),\dots,g_k(x)):\mathbb{R}^n \longrightarrow \mathbb{R}$. Considering $n=1$, we have $f''(x)=g'(x)^\top \nabla h(g(x)) g'(x) + \nabla h(g(x))^\top g''(x)$, then $f(x)$ is convex if $f''(x) \geq 0$ and

f is convex if h is convex and non-decreasing in each argument and g_i are convex
f is convex if h is convex and non-increasing in each argument and g_i are concave
f is concave if h is concave and non-decreasing in each argument and g_i are concave
f is concave if h is concave and non-increasing in each argument and g_i are convex

• Examples of vector composition

- $h(z)=\log(\sum_{i=1,\dots,k} e^{z_i})$ is convex and non-decreasing at each argument, then $\log(\sum_{i=1,\dots,k} e^{g_i(x)})$ is convex whatever $g_i(x)$ is
- If $g_i(x)$ are convex and non-negative, then $(\sum_{i=1,\dots,k} g_i(x)^p)^{1/p}$ is convex

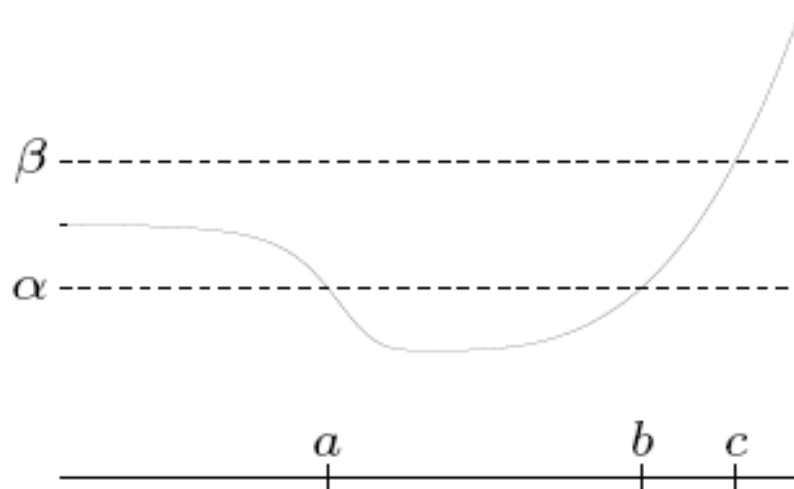
- Quasi-convex functions

A function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is called **quasi-convex** if its domain and all its sublevel sets $S_\alpha = \{x \in \text{dom } f \mid f(x) \leq \alpha\}$ for $\alpha \in \mathbb{R}$ are convex.

Figure: $S_\alpha = [a, b]$ is convex, $S_\beta = (-\infty, c]$ is convex

A function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is called **quasi-concave** if $-f$ is quasi-convex, e.g. superlevel sets $S_\alpha = \{x \in \text{dom } f \mid f(x) \geq \alpha\}$ for $\alpha \in \mathbb{R}$ are convex

A function that is quasi-convex and quasi-concave is called quasi-linear, $S_\alpha = \{x \in \text{dom } f \mid f(x) = \alpha\}$



- **Characterization of quasi-convex functions**

A function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ is **quasi-convex** if its domain f is convex and for any $x_1, x_2 \in \text{dom } f$, we have

$$f(\theta x_1 + (1-\theta)x_2) \leq \max\{f(x_1), f(x_2)\}$$

The value of the function on a segment does not exceed the value at the endpoints.

This is called **Jensen's inequality for quasi-convex functions**

A function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ is **quasi-concave** if its domain f is convex and for any $x_1, x_2 \in \text{dom } f$, we have

$$f(\theta x_1 + (1-\theta)x_2) \geq \min\{f(x_1), f(x_2)\}$$

- **Examples of quasi-convex functions**

- **Logarithm:** $\log x$ on \mathbb{R}_{++} is quasi-linear
- **Ceiling function:** $\text{ceil}(x) = \inf\{z \in \mathbb{Z} \mid z \geq x\}$ is quasi-linear
- **Linear fractional function:** $f(x) = (a^T x + b) / (c^T x + d)$ is quasi-linear in $\text{dom } f = \{x \mid c^T x + d > 0\}$
- $f(x_1, x_2) = x_1 x_2$ is quasi-concave in \mathbb{R}_{++}
- **Distance ratio function:** $f(x) = \|x - a\|_2 / \|x - b\|_2$, then f is quasi-convex on the halfspace $\{x \mid \|x - a\|_2 \leq \|x - b\|_2\}$