Master-MIRI Topics on Optimization and Machine Learning (TOML)

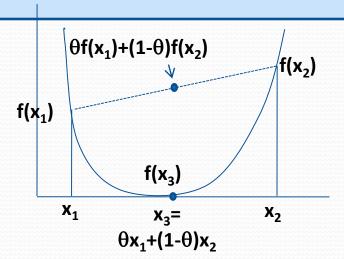
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Domains of a function and Convex Functions

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 $x \in dom f \subset A$ if $f(x) \subset B$ exists.

A function f: $R^n \longrightarrow R$ is convex if

- i. For all $x \in \text{dom } f \subset \mathbb{R}^n$, then dom f is a convex set
- ii. For $0 \le \theta \le 1$, we have $f(\theta x_1 + (1 \theta)x_2) \le \theta f(x_1) + (1 \theta)f(x_2)$
- Strict convexity → change "≤" for "<"
- A function "f" is concave if "-f" is convex
- Affine functions (linear functions) holds equality in condition ii) and thus are both convex and concave



Reminder

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

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

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

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

$$\nabla^2 f(x)_{ij} = \delta f^2(x) / \delta x_1 \delta x_2$$

A matrix A is **positive semi-definite** iif $\forall x$, $x^TAx \ge 0$ (**positive definite** if $x^TAx > 0$). Ways of checking whether a matrix is semi-positive definite is:

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

 all are >0)

A matrix A is **negative semi-definite** iif $\forall x$, $x^TAx \le 0$ (**negative definite** if $x^TAx < 0$). Ways of checking whether a matrix is semi-negative definite is:

- All eigenvalues of A are ≤ 0 (negative definite → all are <0)
- All leading odd principal minors have negative or equal to cero determinants and all even principal minors have positive or equal to cero determinants (negative definite -> 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).

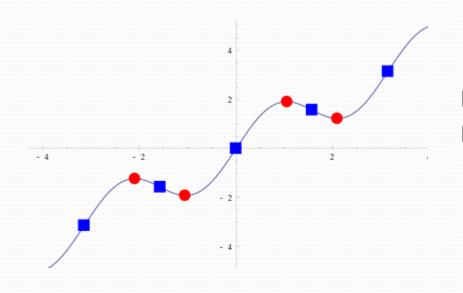
An **inflection point** (is a stationary point) is a point on a curve at which the curvature or concavity changes sign from plus to minus or from minus to plus, i.e., a point on a curve at which the second derivative changes sign and the first derivative is 0.

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.

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

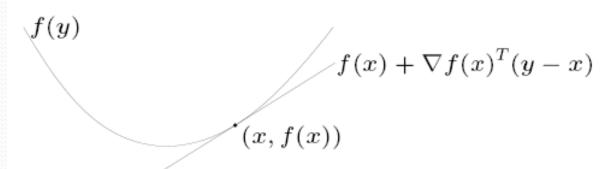
Red dots: maximum or minimum

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 convex
- ii. $f(y) \ge f(x) + \nabla f(x)^T(y-x)$ (first order Taylor approximation of f near x) for all x, y \in \dots om 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: $R^n \longrightarrow R$ be twice differentiable, it is to say the Hessian $\nabla^2 f$ exists in the whole domain of f. Then f is convex iif

- i. dom f is convex
- ii. $\nabla^2 f(x) \ge 0$, the Hessian is semi-definite positive

Be careful, condition i) is necessary: $f(x)=1/x^2$ in 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
- Quadratic functions: $f(x)=\frac{1}{2}x^TPx+q^Tx+r$ are convex for all $P\geq 0$ semi-definite matrix and $x\in R^n$
- Exponential functions: e^{ax} is convex on R and any $a \in R$

• More examples:

- Powers of absolute value $|x|^a$ with a ≥ 1 are convex on R
- Logarithms log x is concave on R++
- Negative entropy x logx is convex on R+ (0log0=0)
- Any norm | | · | |_p is convex on Rⁿ
- Max function, $f(x)=\max\{x_1,x_2,...,x_n\}$ is convex on \mathbb{R}^n
- Quadratic over linear function f(x,y)=x²/y is convex on RxR++
- Log-sum-exp, $f(x)=log(e^{x1}+e^{x2}+...+e^{xn})$ is convex on 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 Sⁿ ++ where Sⁿ ++ is the set of symmetric positive definite nxn matrices

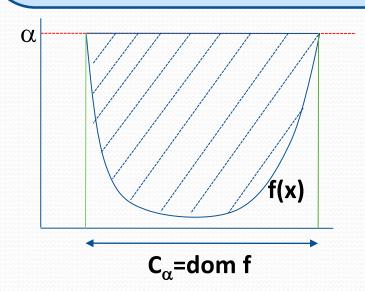
Sub-level sets

A α -sublevel set of a function f: $R^n \longrightarrow R$ 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 $C_{\alpha} = \{x \in \text{dom f } | f(x) \ge \alpha\}$ and are <u>convex.</u> d



Proof:

If
$$x_1, x_2 \in C_\alpha$$
, then $f(x_1) \le \alpha$, $f(x_2) \le \alpha$
Then:

$$f(\theta x_1 + (1-\theta)x_2) \le \theta f(x_1) + (1-\theta)f(x_2) \le \theta \alpha + (1-\theta)\alpha \le \alpha \text{ for } 0 \le \theta \le 1$$

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

- α -level set of a quadratic function:
 - $f(x) = \frac{1}{2}x^TPx$ with P positive definite matrix. Then:

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

Is an ellipsoid with center 0.

• Proof:

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

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:

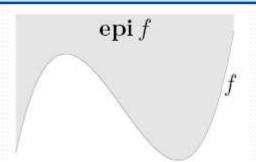
$$E = \{ x \mid \frac{1}{2} (x - x_0)^T P (x - x_0) = \alpha \}$$

Epigraphs/Hypographs

The graph of a function $f: R^n \longrightarrow R$ is defined as

$$\{(x,f(x))| x \in dom f\}$$

The **epigraph** of a function $f: R^n \longrightarrow R$ is defined as epi $f=\{(x,t) \mid x \in \text{dom } f \text{ and } f(x) \leq t\} \subset R^{n+1}$



The **hypograph** of a function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ is defined as $\{(x,t) \mid x \in \text{dom } f \text{ and } f(x) \ge t\} \subset \mathbb{R}^{n+1}$

A function is convex iif its epigraph is a convex set

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

$$f(\theta_1 x_1 + \theta_2 x_2 + ... + \theta_k x_k) \le \theta_1 f(x_1) + \theta_1 f(x_1) + ... + \theta_k f(x_k)$$

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

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

Linear functions and affine functions

In **analytic geometry**, <u>a linear function</u> is a polynomial: e.g. in one dimension f(x) = ax+b or in more dimensions $f(x_1, ...x_n) = a_1x_1 + ... + a_nx_n$ is a hyperplane.

In **linear algebra**, <u>a linear function (or linear map)</u> 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).

Conjugate Function

The function $f^*: R^n \to R$ 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.

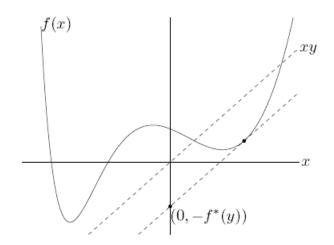


Figure 3.8 A function $f: \mathbf{R} \to \mathbf{R}$, and a value $y \in \mathbf{R}$. The conjugate function $f^*(y)$ is the maximum gap between the linear function yx and f(x), as shown by the dashed line in the figure. If f is differentiable, this occurs at a point x where f'(x) = y.

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

$$f^*(y) = \sup_{x} (\langle x, y \rangle - f(x)) = \sup_{x} (y^T x - f(x))$$

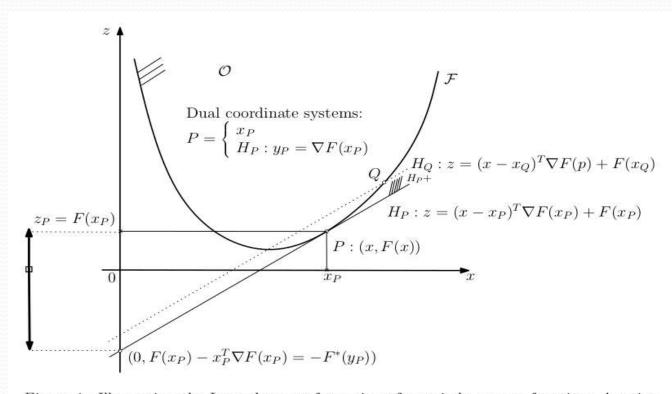


Figure 1: Illustration the Legendre transformation of a strictly convex function: A point P on the boundary of \mathcal{O} can either be parameterized by using the x-coordinate system, or by using the dual slope $y = \nabla F(x)$ coordinate system. For a point $P \in \partial O$ with x-coordinate x_P , 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 x-axis. The object x-object x-ob

Conjugate Function

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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 iif f is convex and closed (i.e. 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 dom $f^*=R+$
 - Negative entropy: $f(x)=x\log(x) \rightarrow f^*(y)=e^{y-1}$ with dom $f^*=R$
 - Indicator function: $f_S(x)=0$ if $x \in S \rightarrow f^*(y)=\sup_x (y^Tx)$
 - Log-sum-exp: $f(x)=log(\Sigma_{i=1..m} exp(x_i)) \rightarrow f^*(y)=\Sigma_{i=1..m} y_i log(y_i)$ with $\mathbf{1}^T y$ =1 and $y \ge 0$

Operations that preserve convexity

- Non-negative weighted sums: $f=w_1f_1+...+w_mf_m$ is convex if f_i is convex and $w_i \ge 0$ for i=1,...,m
- Non-negative weighted integrals: $g(x)=\int_A w(y)f(x,y)dy$ is convex if f(x,y) convex in x and $w(y)\geq 0$ for each $y\in A$
- Composition with an affine mapping: $f:R^n \longrightarrow R$, $A \in R^{nxm}$, $b \in R^n$, and let be $g:R^n \longrightarrow R$ such as g(x)=f(Ax+b) with dom $g=\{x \mid Ax+b \in dom f\}$. Then, if f is convex (concave), so is g.
- Pointwise maximum: g(x)=max{f₁(x),...,f_m(x)} is convex if f_i is convex for i=1,...,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, dom $g=\{x\mid (x,y)\in dom\ f$ for all $y\in A$, $\sup_{y\in A}\{f(x,y)\}<\infty\}$.

Composition

- Let be $h:R^k \longrightarrow R$ and $g:R^n \longrightarrow R^k$ functions, and let us consider composition $f=h^\circ g=h(g(x)): R^n \longrightarrow R$, with dom $f=\{x \in dom \ g \mid g(x) \in dom \ h\}$.
- Let us consider the cases, k=1 and n=1, h:R \longrightarrow R, g:R \longrightarrow R and remember than 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, $f''(x)\ge 0$

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

Vector Composition

• Let us now consider $h: R^k \longrightarrow R$ and $g_i: R^n \longrightarrow R$ functions, and let us consider composition $f=h(g_1(x),...,g_k(x)): R^n \longrightarrow R$. Considering n=1, we have $f''(x)=g'(x)^T \nabla h(g(x)) \ g'(x) + \nabla h(g(x))^T \ g''(x)$, then f(x) is convex if $f''(x) \ge 0$ 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

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

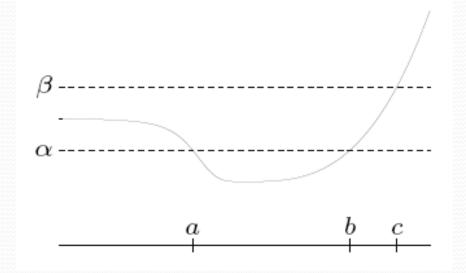
Quasi-convex functions

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

Figure: S_{α} =[a,b] is convex, S_{β} =(-\infty,c] is convex

A function $f:R^n \longrightarrow R$ is called **quasi-concave** if -f is quasi-convex, e.g. superlevel sets $S_\alpha = \{x \in \text{dom } f \mid f(x) \ge \alpha\}$ for $\alpha \in R$ 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 $f:R^n \longrightarrow R$ is **quasi-convex** if its domain f is convex and for any $x_1, x_2 \in dom f$, we have

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

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

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

- Examples of quasi-convex functions
 - Logarithm: log x on R++ is quasi-linear
 - Ceiling function: $ceil(x)=\inf\{z\in Z\mid z\geq x\}$ is quasi-linear
 - Linear fractional function: $f(x) = (a^Tx+b)/(c^Tx+d)$ is quasi-linear in dom $f=\{x \mid c^Tx+d>0\}$
 - $f(x_1,x_2)=x_1x_2$ is quasi-concave in R++
 - Distance ratio function: $f(x)=||x-a||_2/||x-b||_2$, then f is quasi-convex on the halfspace $\{x \mid ||x-a||_2 \le ||x-b||_2\}$