Introduction to Optimization

Lecture 5: Continuous Optimization II

October 16, 2015

TC2 - Optimisation

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Course Overview

Date		Topic
Fri, 18.9.2015	DB	Introduction and Greedy Algorithms
Fri, 25.9.2015	DB	Dynamic programming and Branch and Bound
Fri, 2.10.2015	DB	Approximation Algorithms and Heuristics
Fri, 9.10.2015	AA	Introduction to Continuous Optimization
Fri, 16.10.2015	AA	End of Intro to Cont. Opt. + Gradient-Based Algorithms I
Fri, 30.10.2015	AA	Gradient-Based Algorithms II
Fri, 6.11.2015	AA	Stochastic Algorithms and Derivative-free Optimization
16 - 20.11.2015		Exam (exact date to be confirmed)

all classes + exam are from 14h till 17h15 (incl. a 15min break)
here in PUIO-D101/D103

Further Details on Remaining Lectures

Introduction to Continuous Optimization

- examples (from ML / black-box problems)
- typical difficulties in optimization

Mathematical Tools to Characterize Optima

- reminders about differentiability, gradient, Hessian matrix
- unconstraint optimization
  - first and second order conditions
  - convexity
- constraint optimization

Gradient-based Algorithms

- quasi-Newton method (BFGS)
- DFO trust-region method

Learning in Optimization / Stochastic Optimization

- CMA-ES (adaptive algorithms / Information Geometry)
- PhD thesis possible on this topic

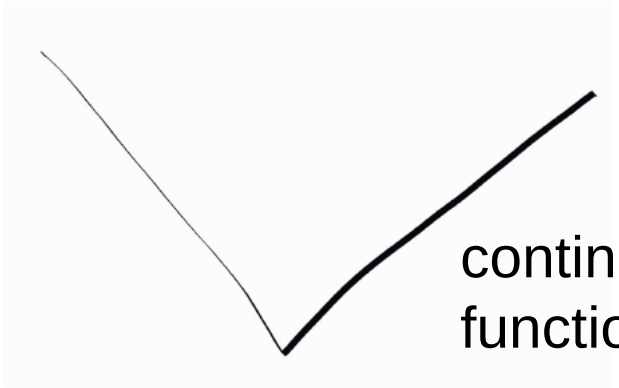
method strongly related to ML / new promising research area

interesting open questions

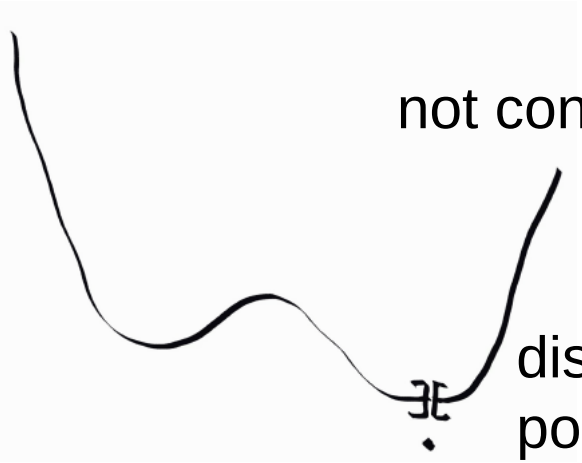
Continuity of a Function

$f: (E, ||\quad||) \longrightarrow (E, ||\quad||)$ is continuous in $x \in E$ if

$\forall \epsilon > 0, \exists \eta > 0$ such that $\forall y$: $||x - y|| \leq \eta; ||f(x) - f(y)|| \leq \epsilon$



continuous function



not continuous

discontinuity point

Scalar Product

$\langle , \rangle : E \times E \to \mathbb{R}$ is a scalar product if it is

- a bilinear application
- symmetric (i.e. $\langle x, y \rangle = \langle y, x \rangle$
- positive (i.e. $\forall x \in E$: $\langle x, x \rangle \geq 0$)
- definite (i.e. $\langle x, x \rangle = 0 \implies x = 0$)

Given a scalar product $\langle \ , \ \rangle$, $||x|| = \sqrt{\langle x, x \rangle}$ is a norm.

(home exercise)

Example in $\mathbb{R}^n$: $\langle x, y \rangle = x^T y$

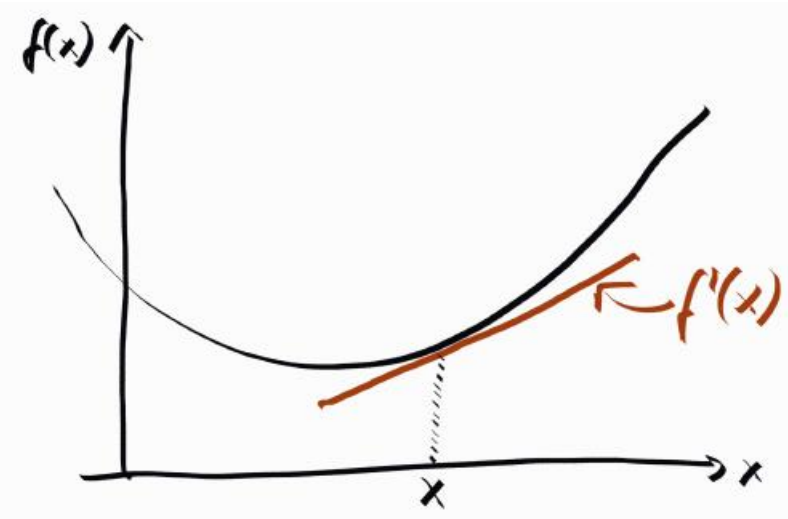
Reminder: Derivability in 1D (n=1)

$f: \mathbb{R} \to \mathbb{R}$ is derivable in $x \in \mathbb{R}$ if

$$\lim_{h \to 0} \frac{f(x+h)-f(x)}{h} \text{ exists, } h \in \mathbb{R}$$

Notation:

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



The derivative corresponds to the slope of the tangent in x.

Reminder: Derivability in 1D (n=1)

Taylor Formula (Order 1)

If f is derivable in x then

$$f(x+h) = f(x) + f'(x)h + o\left(||h||\right)$$

i.e. for h small enough, $h \longmapsto f(x+h)$ is approximated by $h \longmapsto f(x) + f'(h)$

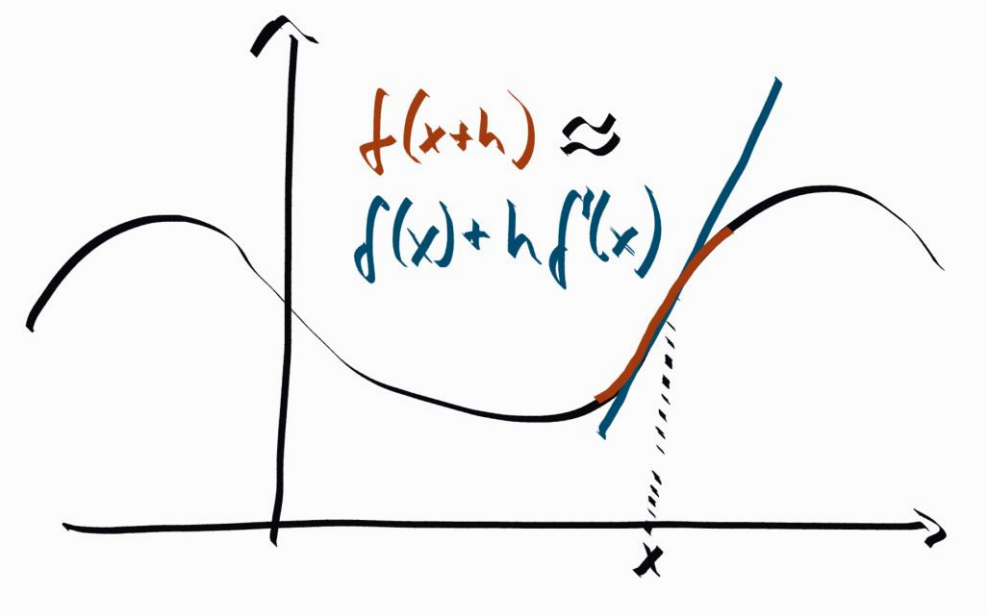
$h \longmapsto f(x) + f'(x)h$ is a linear approximation of $f(x+h)$

Exercise:
Why is it linear?

$h \longmapsto f(x) + f'(x)h$ is a first order approximation of $f(x+h)$

Reminder: Derivability in 1D (n=1)

Geometrically:



The notion of derivative of a function defined on $\mathbb{R}^n$ is generalized via this idea of a linear approximation of $f(x+h)$ for h small enough.

Differentiability: Generalization from 1D

Given a normed vector space $(E, ||.||)$ and complete (Banach space), consider $f: U \subset E \to \mathbb{R}$ with U open set of E.

- f is differentiable in $\boldsymbol{x} \in U$ if there exists a continuous linear mapping $Df(\boldsymbol{x})$ such that

$$f(\boldsymbol{x} + \boldsymbol{h}) = f(\boldsymbol{x}) + Df(\boldsymbol{x})(\boldsymbol{h}) + o(||\boldsymbol{h}||)$$

$Df(\boldsymbol{x})$ is the differential of f in $\boldsymbol{x}$

Exercise:

Consider $E = \mathbb{R}^n$ with the scalar product $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^T \boldsymbol{y}$. Let $\boldsymbol{a} \in \mathbb{R}^n$, show that

$$f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle$$

is differentiable and compute its differential.

Gradient

If the norm $||.||$ comes from a scalar product, i.e. $||\boldsymbol{x}|| = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$ (the Banach space E is then called a Hilbert space), the gradient of f in $\boldsymbol{x}$ denoted $\nabla f(\boldsymbol{x})$ is defined as the element of E such that

$$Df(\boldsymbol{x})(\boldsymbol{h}) = \langle \nabla f(\boldsymbol{x}), \boldsymbol{h} \rangle$$

Riesz representation Theorem

Taylor formula – order one

Replacing the differential in the last slide by the above, we obtain the Taylor formula:

$$f(\boldsymbol{x} + \boldsymbol{h}) = f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{h} \rangle + o(||\boldsymbol{h}||)$$

Exercise: Gradients

Exercise:

Compute the gradient of the functions

- $f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle$.
- $f_n(\theta) = \frac{1}{2}(y_n - \langle \Phi(\boldsymbol{x}_n), \theta \rangle)^2$.

Gradient: Connection to Partial Derivatives

- In $(\mathbb{R}^n, \ ||\quad||_2)$ where $||\boldsymbol{x}||_2 = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$ is the Euclidean norm deriving from the scalar product $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^T \boldsymbol{y}$

$$\nabla f(x) = \begin{pmatrix} \dfrac{\partial f}{\partial x_1} \\ \vdots \\ \dfrac{\partial f}{\partial x_n} \end{pmatrix}$$

- Reminder: partial derivative in x_0

$$y \underset{f_i}{\rightarrow} f\left(x_0^1, \ldots, x_0^{i-1}, y, x_0^{i+1}, \ldots, x_0^n\right)$$

$$\frac{\partial \mathrm{f}}{\partial x_i}(x_0) = f_i{}'(x_0)$$

Gradient: More Examples

- if $f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle, \nabla f(x) = \boldsymbol{a}$
- in $\mathbb{R}^n$, if $f(\boldsymbol{x}) = \boldsymbol{x}^T A \boldsymbol{x}$, then $\nabla f(\boldsymbol{x}) = (A + A^T)\boldsymbol{x}$
- particular case if $f(\boldsymbol{x}) = ||\boldsymbol{x}||^2$, then $\nabla f(\boldsymbol{x}) = 2\boldsymbol{x}$
- in $\mathbb{R}$, $\nabla f(\boldsymbol{x}) = f'(\boldsymbol{x})$

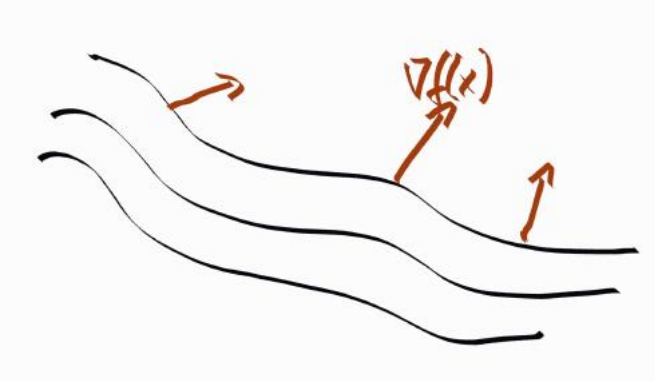
Gradient: Geometrical Interpretation

Exercise:

Let $L_c = \{\boldsymbol{x} \in \mathbb{R}^n \mid f(\boldsymbol{x}) = c\}$ be again a level set of a function $f(\boldsymbol{x})$.
Let $\boldsymbol{x}_0 \in L_c \neq \emptyset$.

Show for $f(\boldsymbol{x}) = \langle \boldsymbol{a}, \boldsymbol{x} \rangle$ and $f(\boldsymbol{x}) = ||\boldsymbol{x}||^2$ that $\nabla f(\boldsymbol{x_0})$ is ***orthogonal*** to the level sets in x_0.

More generally, the gradient of a differentiable function is orthogonal to its level sets.

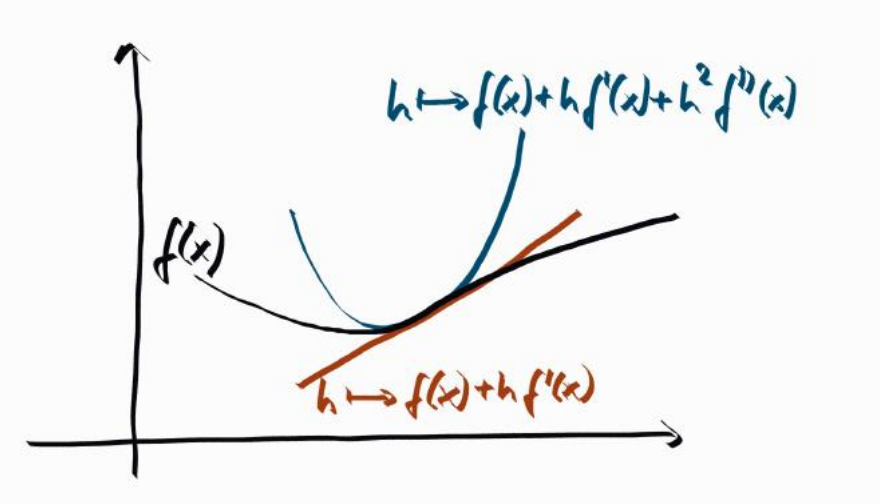


Reminder: Second Order Derivability in 1D

- Let $f: \mathbb{R} \to \mathbb{R}$ be a derivable function and let $f': x \to f'(x)$ be its derivative function.
- If f' is derivable in x, then we denote its derivative as $f''(x)$
- $f''(x)$ is called the *second order derivative* of f.

Taylor Formula: Second Order Derivative

- If $f: \mathbb{R} \to \mathbb{R}$ is two times derivable then
$$f(x+h) = f(x) + f'(x)h + f''(x)h^2 + o(||h||^2)$$
i.e. for h small enough, $h \to f(x) + hf'(x) + h^2 f''(x)$ approximates $h + f(x+h)$
- $h \to f(x) + hf'(x) + h^2 f''(x)$ is a quadratic approximation (or order 2) of f in a neighborhood of x



- The second derivative of $f: \mathbb{R} \to \mathbb{R}$ generalizes naturally to larger dimension.

Second Order Differentiability

- (first order) differential: gives a linear local approximation
- second order differential: gives a quadratic local approximation

Definition: second order differentiability

$f: U \subset E \to \mathbb{R}$ is differentiable at the second order in $\boldsymbol{x} \in U$ if it is differentiable in a neighborhood of $\boldsymbol{x}$ and if $u \longmapsto Df(u)$ is differentiable in $\boldsymbol{x}$

Second Order Differentiability (Cont.)

Another Definition:

$f: U \subset E \to \mathbb{R}$ is differentiable at the second order in $\boldsymbol{x} \in U$ iff there exists a continuous linear application $Df(\boldsymbol{x})$ and a bilinear symmetric continuous application $D^2 f(\boldsymbol{x})$ such that

$$f(\boldsymbol{x}+\boldsymbol{h}) = f(\boldsymbol{x}) + Df(\boldsymbol{x})(\boldsymbol{h}) + \frac{1}{2} D^2 f(\boldsymbol{x})(\boldsymbol{h},\boldsymbol{h}) + o(||\boldsymbol{h}||^2)$$

In a Hilbert space $(E, \langle \quad \rangle)$

$$D^2 f(\boldsymbol{x})(\boldsymbol{h},\boldsymbol{h}) = \langle \nabla^2 f(\boldsymbol{x})(\boldsymbol{h}), \boldsymbol{h} \rangle$$

where $\nabla^2 f(\boldsymbol{x})$: $E \to E$ is a symmetric continuous operator.

Hessian Matrix

In $(\mathbb{R}^n, \langle x, y \rangle = x^T y)$, $\nabla^2 f(x)$ is represented by a symmetric matrix called the Hessian matrix. It can be computed as

$$\nabla^2(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Exercise on Hessian Matrix

Exercise:

Let $f(\boldsymbol{x}) = \boldsymbol{x}^T A\, \boldsymbol{x}$, $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$.

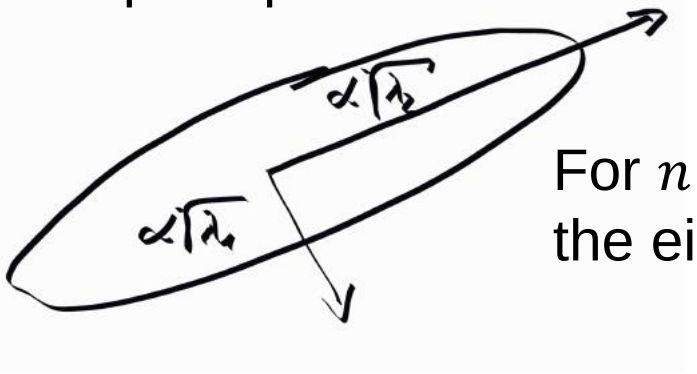
Compute the Hessian matrix of f.

If it is too complex, consider f: $\begin{cases} \mathbb{R}^2 \to \mathbb{R} \\ \boldsymbol{x} \to \boldsymbol{x}^T A\, \boldsymbol{x} \end{cases}$ with $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}$

Back to Ill-Conditioned Problems

We have seen that for a convex quadratic function $f(x) = \frac{1}{2}(x - x_0)^T A(x - x_0) + b$ of $x \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$, A SPD, $b \in \mathbb{R}^n$:

1) The level sets are ellipsoids. The eigenvalues of A determine the lengths of the principle axes of the ellipsoid.



For $n = 2$, let λ_1, λ_2 be the eigenvalues of A.

2) The Hessian matrix of f equals to A.

Ill-conditioned convex quadratic problems are problems with large ratio between largest and smallest eigenvalue of A which means large ratio between longest and shortest axis of ellipsoid.

This corresponds to having an ill-conditioned Hessian matrix.

Optimality Conditions: First Order Necessary Cond.

For 1-dimensional optimization problems f: $\mathbb{R} \to \mathbb{R}$

Assume f is derivable

- $\boldsymbol{x}^*$ is a local extremum $\Longrightarrow f'(\boldsymbol{x}^*) = 0$

not a sufficient condition: consider $f(\boldsymbol{x}) = \boldsymbol{x}^3$

proof via Taylor formula: $f(\boldsymbol{x}^* + \boldsymbol{h}) = f(\boldsymbol{x}^*) + f'(\boldsymbol{x}^*)h + o(||\boldsymbol{h}||)$

- points $\boldsymbol{y}$ such that $f'(\boldsymbol{y}) = 0$ are called critical or stationary points

Generalization to n-dimensional functions

If $f: U \subset \mathbb{R}^n \longmapsto \mathbb{R}$ is differentiable

- necessary condition: If $\boldsymbol{x}^*$ is a local extremum of f, then $Df(\boldsymbol{x}^*) = 0$ and hence $\nabla f(\boldsymbol{x}^*) = 0$

proof via Taylor formula

Second Order Necessary and Sufficient Opt. Cond.

If f is twice continuously differentiable

- Necessary condition: if $\boldsymbol{x}^*$ is a local minimum, then $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semi-definite

proof via Taylor formula at order 2

- Sufficient condition: if $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive definite, then $\boldsymbol{x}^*$ is a strict local minimum

Proof for sufficient condition:

- Let $\lambda > 0$ be the smallest eigenvalue of $\nabla^2 f(\boldsymbol{x}^*)$, using a second order Taylor expansion, we have for all $\boldsymbol{h}$:
- $$f(\boldsymbol{x}^* + \boldsymbol{h}) - f(\boldsymbol{x}^*) = \nabla f(\boldsymbol{x}^*)^T \boldsymbol{h} + \frac{1}{2} \boldsymbol{h}^T \nabla^2 f(\boldsymbol{x}^*) \boldsymbol{h} + o(||\boldsymbol{h}||^2)$$
$$> \frac{\lambda}{2} ||\boldsymbol{h}||^2 + \mathrm{o}(||\boldsymbol{h}||^2) = \left(\frac{\lambda}{2} + \frac{o(||\boldsymbol{h}||^2)}{||\boldsymbol{h}||^2} \right) ||\boldsymbol{h}||^2$$

Convex Functions

Let U be a convex open of $\mathbb{R}^n$ and $f: U \to \mathbb{R}$. The function f is said to be convex if for all $\boldsymbol{x}, \boldsymbol{y} \in U$ and for all $t \in [0,1]$

$$f\big((1-t)\boldsymbol{x} + t\boldsymbol{y}\big) \leq (1-t)f(\boldsymbol{x}) + tf(\boldsymbol{y})$$

Theorem

If f is differentiable, then f is convex if and only if for all $\boldsymbol{x}, \boldsymbol{y}$

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq Df(\boldsymbol{x})(\boldsymbol{y} - \boldsymbol{x})$$

if $n = 1$, the curve is on top of the tangent

If f is twice continuously differentiable, then f is convex if and only if $D^2 f$ satisfies $\forall \boldsymbol{x} \in U, \boldsymbol{h} \in \mathbb{R}^n: D^2 f(\boldsymbol{x})(\boldsymbol{h}, \boldsymbol{h}) \geq 0$ (or $\nabla^2 f(\boldsymbol{x})$ is positive semi-definite for all x)

Convex Functions: Why Convexity?

Examples:

- $f(\boldsymbol{x}) = \langle a, \boldsymbol{x} \rangle + b$
- $f(\boldsymbol{x}) = \frac{1}{2}\langle \boldsymbol{x}, A\boldsymbol{x} \rangle + \langle a, \boldsymbol{x} \rangle + b$, A positive definite symmetric

the opposite of the entropy function: $f(\boldsymbol{x}) = -\sum_{i=1}^{n} \boldsymbol{x}_i \ln(\boldsymbol{x}_i)$ (the entropy function is then concave)

Exercise:

Let $f: U \to \mathbb{R}$ be a convex and differentiable function on a convex open U.
Show that if $Df(\boldsymbol{x}^*) = 0$, then $\boldsymbol{x}^*$ is a global minimum of f

Why convexity? local minima are also global under convexity assumption.