Extreme values: Convexity.

Discrete Mathematics and Optimization
Bioinformatics

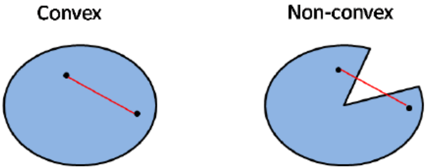
1. Convex sets

When local extrema can be ensured to be global?

Convexity is an important notion

Definition

A subset $C \subset \mathbb{R}^n$ is convex if, for every $\mathbf{x}, \mathbf{y} \in C$, C contains all points in the segment joining $\mathbf{x}$ and $\mathbf{y}$.



For every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ the segment joining $\mathbf{x}$ and $\mathbf{y}$ consists of the points

$$\lambda \mathbf{x} + (1-\lambda)\mathbf{y},\ 0\ le \lambda \leq 1.$$

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Examples of convex sets

- Balls $B(\mathbf{x}, r) = \{\mathbf{y} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{y}\| \leq r\}$ are convex.
- Translates of vector subspaces of $\mathbb{R}^n$ are convex (lines, planes,...)
- If $C_1, C_2 \subset \mathbb{R}^n$ are convex then $C_1 \cap C_2$ is convex.
- Polytopes (constraints in Linear Programming) are convex.
- If $S = \{x_1, \ldots, x_k\} \subset \mathbb{R}^n$, the convex hull of S

$$Conv(S) = \{\lambda_1 x_1 + \cdots + \lambda_k x_k : \lambda_i \geq 0, \lambda_1 + \cdots + \lambda_k = 1\},$$

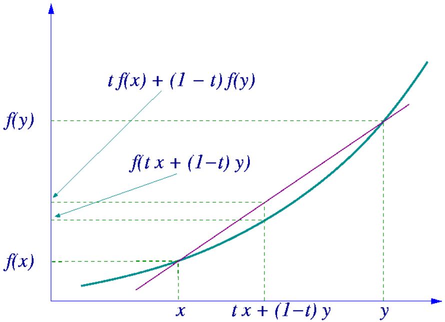
is convex.

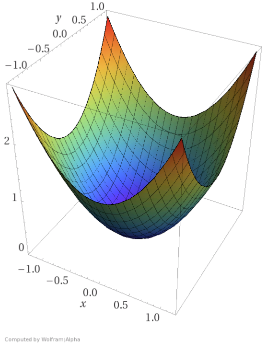
2. Convex functions

Definition

A function $f : C \subset \mathbb{R}^n \to \mathbb{R}$ is convex on the convex set C if, for every $\mathbf{x}, \mathbf{y} \in C$ and all $0 \leq \lambda \leq 1$,

$$f(\lambda \mathbf{x} + (1-\lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1-\lambda) f(\mathbf{y}).$$





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- Strict convex if the inequality is strict.
- Concave if the opposite inequality holds.
- $f(\mathbf{x})$ is convex if and only if $-f(\mathbf{x})$ is concave.
- If f is convex on C and $\lambda_1 + \cdots + \lambda_k = 1$, $\lambda_i \geq 0$ then, for every $\mathbf{x}_1, \ldots, \mathbf{x}_k \in C$,

$$f(\lambda_1 \mathbf{x}_1 + \cdots \lambda_k \mathbf{x}_k) \leq \lambda_1 f(\mathbf{x}_1) + \cdots + \lambda_k f(\mathbf{x}_k).$$

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Why convexity is important in optimization?

Theorem

Let $f : C \subset \mathbb{R}^n \to \mathbb{R}$ be a convex function on the convex set C.
Then a (strict) local minimum of f is a (strict) global one.

- Let $\mathbf{x}_0$ be a local minimum, $f(\mathbf{x}_0) \leq f(\mathbf{y})$ for all $\mathbf{y}$ close to $\mathbf{x}_0$.
- Let $\mathbf{x} \in C$. Choose $0 < \lambda < 1$ such that $(1-\lambda)\mathbf{x}_0 + \lambda \mathbf{x}$ is close to $\mathbf{x}_0$.
- By convexity, $f(\mathbf{x}_0) \leq f((1-\lambda)\mathbf{x}_0 + \lambda \mathbf{x}) \leq (1-\lambda) f(\mathbf{x}_0) + \lambda f(\mathbf{x})$.
- It follows that $f(\mathbf{x}_0) \leq f(\mathbf{x})$.

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A word of caution

If f is convex its global minimum is contained in the critical points $(\nabla f(\mathbf{x}) = 0)$ or on the boundary of C.

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Examples of convex functions:

- Linear functions $f(x_1, \ldots, x_n) = a_1 x_1 + \cdots + a_n x_n$ are convex (and concave).
- $x^2, x^4, \cdots$ are convex.
- Odd powers $x^3, x^5, \ldots$ are not convex in $\mathbb{R}$.
- Exponential e^x is convex.
- Logarithm $\log(x)$ is concave.

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How to check if f is convex?

Theorem

Let $f \in \mathcal{C}^2(C)$. Then f is f is convex on C if and only if the Hessian matrix of f is positive semidefinite at every point $x \in C$.

Example: $f(x,y) = x^2 - xy + y^2$

- $\nabla f(x,y) = (2x - y, 2y - x)$
- $Hf(x,y) = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$

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An idea of the proof.

- f is convex if and only if $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x})$.
- Use quadratic approximation
  $f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}) + (\mathbf{y} - \mathbf{x})^T Hf(\mathbf{x})(\mathbf{y} - \mathbf{x}) + o(\|\mathbf{y} - \mathbf{x}\|^2)$.

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How to check if f is convex?

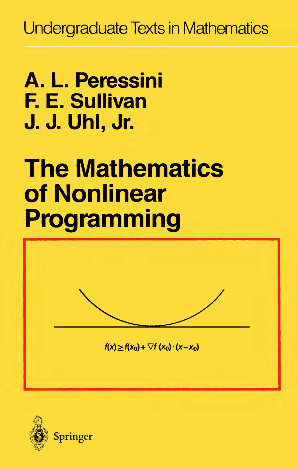
- If $f_1(\mathbf{x}), f_2(\mathbf{x})$ are convex on C then $f(\mathbf{x}) = f_1(\mathbf{x}) + f_2(\mathbf{x})$ is convex on C.
- If $f(\mathbf{x})$ is convex on C and $\alpha \in \mathbb{R}$, $\alpha > 0$, then $(\alpha f)(\mathbf{x})$ is convex on C.
- If f is convex on C and $g : f(C) \subset \mathbb{R} \to \mathbb{R}$ is increasing then $g(f(\mathbf{x}))$ is convex on C.

Example: $f(x, y) = e^{(x^2+y^2)} - \log(xy)$ is convex.

Summary

- Convex functions on convex sets have a global minimum if they have a local one.
- Convexity of a function can be discovered either by analyzing its components or by positivity of the Hessian.
- Convex optimization is a large area including topics as:
  - Least squares
  - Linear programming
  - Convex quadratic minimization with linear constraints
  - Quadratic minimization with convex quadratic constraints
  - Geometric programming
  - Semidefinite programming
  - Entropy maximization with appropriate constraints
  - ....

A reference



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