Optimization Preliminaries

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Introduction

Optimization Problem Setting

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Our aim is to find a minimum for the function f in the set $\mathcal{X}$.
This is called an optimization problem.

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- Deterministic (all problem parameters are assumed to be exactly known) *vs* stochastic (some parameters are random variables),
- Mono-objective ($f(\mathbf{x}) \in \mathbb{R}$) *vs* multi-objective ($f(\mathbf{x}) \in \mathbb{R}^m$),
- Convex ($f(\mathbf{x})$ is a convex function and $\mathcal{X}$ is a convex set) *vs* Non-convex ($f(\mathbf{x})$ is a non-convex function or $\mathcal{X}$ is a non-convex set).

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Thus, the formulation given above remains valid for any optimization problem.

Local and global minima

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A point $\mathbf{x}$ is said to be a **local minimum**(resp. **local maximum**) of f in $\mathcal{X}$, if $f(\mathbf{x}) \leq f(\mathbf{y})$ (resp. $f(\mathbf{x}) \geq f(\mathbf{y})$) for all $\mathbf{y}$ in some neighborhood $N \subseteq \mathcal{X}$ about $\mathbf{x}$.

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Furthermore, if $f(\mathbf{x}) \leq f(\mathbf{y})$ for all $\mathbf{y} \in \mathcal{X}$, then $\mathbf{x}$ is a **global minimum** of f in $\mathcal{X}$ (similarly for global maximum).

Conditions for local minima

First order necessary condition

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If $\mathbf{x}^*$ is a local minimum of f and f is continuously differentiable in a neighborhood of $\mathbf{x}^*$, then $\nabla f(\mathbf{x}^*) = \mathbf{0}$.

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Thus there exists $\beta > 0$ such that $\mathbf{h}^\top \nabla f(\mathbf{x}^* + \alpha \mathbf{h}) < 0$ for all $\alpha \in [0, \beta]$.

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whence it follows that x^* is not a local minimum, a contradiction. Hence $\nabla f(\mathbf{x}^*) = 0$.

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If $\nabla f(\mathbf{x})$ is nonzero, there always exists a sufficiently small step $\alpha > 0$ such that $f(\mathbf{x} - \alpha \nabla f(\mathbf{x})) < f(\mathbf{x})$. For this reason, $-\nabla f(\mathbf{x})$ is called a **descent direction.**

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Points where the gradient vanishes are called **stationary points.**

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For example, consider $f : \mathbb{R}^2 \to \mathbb{R}$ given by $f(x, y) = x^2 - y^2$.

We have $f(\mathbf{0}) = \mathbf{0}$, but the point $\mathbf{0}$ is the minimum along the line $y = 0$ and the maximum along the line $x = 0$.

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We have $f(\mathbf{0}) = \mathbf{0}$, but the point $\mathbf{0}$ is the minimum along the line $y = 0$ and the maximum along the line $x = 0$.

Thus it is neither a local minimum nor a local maximum of f.

Points such as these, where the gradient vanishes but there is no local extremum, are called **saddle points**.

Second order necessary condition

Second order necessary condition

A second-order necessary condition (i.e. the Hessian) for existence of local minima is given:

Proposition

If $\mathbf{x}^*$ is a local minimum of f and f is twice continuously differentiable in a neighborhood of $\mathbf{x}^*$, then $\nabla^2 f(\mathbf{x}^*)$ is positive semi-definite.

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Proposition

Suppose f is twice continuously differentiable with $\nabla^2 f$ positive semi-definite in a neighborhood of $\mathbf{x}^*$, and that $\nabla f(\mathbf{x}^*) = \mathbf{0}$. Then $\mathbf{x}^*$ is a local minimum of f. Furthermore if $\nabla^2 f(\mathbf{x}^*)$ is positive definite, then $\mathbf{x}^*$ is a strict local minimum.

Proof

Let B be an open ball of radius $r > 0$ centered at $\mathbf{x}^*$ which is contained in the neighborhood. Applying Taylor's theorem, we have that for any $\mathbf{h}$ with $\|\mathbf{h}\|_2 < r$, there exists $t \in (0;1)$ such that

$$f(\mathbf{x}^* + \mathbf{h}) = f(\mathbf{x}^*) + \underbrace{\mathbf{h}^\top \nabla f(\mathbf{x}^*)}_{=0} + \frac{1}{2} \underbrace{\mathbf{h}^\top \nabla^2 f(\mathbf{x}^* + t\mathbf{h})\mathbf{h}}_{\geq 0} \geq f(\mathbf{x}^*)$$

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Therefore, $\mathbf{x}^*$ is a local minimum of f.
Now, if $\nabla^2 f$ is definite positive then $\mathbf{h}^\top \nabla^2 f(\mathbf{x}^* + t\mathbf{h})\mathbf{h} > 0$ and thus $\mathbf{x}^*$ is a strict local minimum.

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For these reasons we require that the Hessian remains positive semi-definite as long as we are close to $\mathbf{x}^*$.
This condition is not practical to check computationally, but in some cases we can verify it analytically (usually by showing that $\nabla^2 f(\mathbf{x})$ is p.s.d. for all $\mathbf{x} \in \mathbb{R}^d$).

Convexity

Introduction

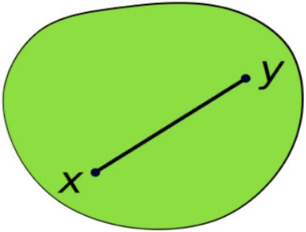
Convexity is a term that pertains to both sets and functions.

Convex sets

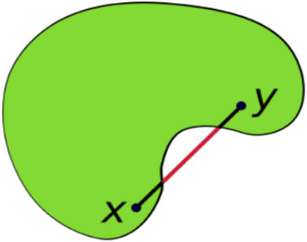
A set $\mathcal{X} \subseteq \mathbb{R}^d$ is convex if for all $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ and all $t \in [0, 1]$

$$t\mathbf{x} + (1 - t)\mathbf{y} \in \mathcal{X}$$

Geometrically, this means that all the points on the line segment between any two points in $\mathcal{X}$ are also in $\mathcal{X}$.



(a) A convex set



(b) A non-convex set

Convex functions

For functions, there are different degrees of convexity, and how convex a function is, tells us a lot about its minima: do they exist, are they unique, how quickly can we find them using optimization algorithms, etc.

A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if

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

for all $\mathbf{x}, \mathbf{y} \in \operatorname{dom} f$ and all $t \in [0,1]$.
If the inequality above holds strictly for all $t \in [0,1]$ and $\mathbf{x} \neq \mathbf{y}$, then we say that f is said **strictly convex**.

A function f is **strongly convex with parameter** m (or m**-strongly convex**) if the function

$$\mathbf{x} \mapsto f(\mathbf{x}) - \frac{m}{2}\|\mathbf{x}\|_2^2$$

is convex. i.e :

$$f(t\mathbf{x} + (1-t)\mathbf{y}) \leq tf(\mathbf{x}) + (1-t)f(\mathbf{y}) + \frac{m}{2}t(1-t)\|\mathbf{x} - \mathbf{y}\|_2^2$$

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These conditions are given in increasing order of strength; strong convexity implies strict convexity which implies convexity.

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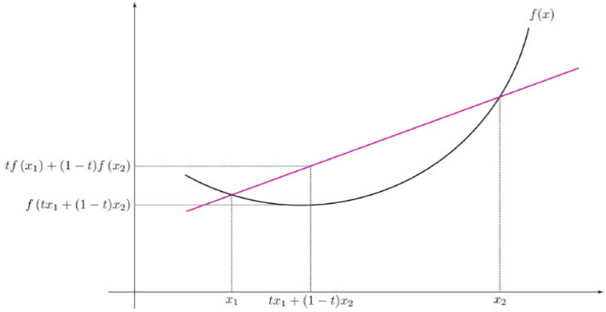

Characterization of convex, strictly convex and strongly convex functions

It is usually not easy to verify that the (strict, strong)-convexity of a given function from the definition. But the following theorems give us another way to do that.

Theorem

Suppose f is differentiable. Then

- *f is convex if and only if*

$$f(\mathbf{x}) \geq f(\mathbf{y}) + \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle, \text{ for all } \mathbf{x}, \mathbf{y} \in \operatorname{dom} f$$

- *f is strictly convex if and only if*

$$f(\mathbf{x}) > f(\mathbf{y}) + \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle, \text{ for all } \mathbf{x}, \mathbf{y} \in \operatorname{dom} f, \mathbf{x} \neq \mathbf{y}$$

- *f is m-strongly convex if and only if*

$$f(\mathbf{x}) \geq f(\mathbf{y}) + \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle + \frac{m}{2} \|y - x\|_2^2$$

Theorem

Suppose f is twice differentiable. Then

- *f is convex if and only if $\nabla^2 f(\mathbf{x})$ is positive semi definite for all $\mathbf{x} \in \operatorname{dom} f$*
- *If $\nabla^2 f(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \operatorname{dom} f$ then f is strictly convex.*
- *f is m-strongly convex if and only if $\nabla^2 f(\mathbf{x}) - mI$ is positive semidefinite for all $\mathbf{x} \in \operatorname{dom} f$.*

Properties of convex functions

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3. If $f_1, f_2, \ldots, f_k$ are convex and $\alpha_1, \alpha_2, \ldots, \alpha_k > 0$ then $f = \sum_{i=1}^{k} \alpha_i f_i$ is convex.

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4. If f is convex, then $g(\mathbf{x}) \equiv f(\mathbf{A}\mathbf{x} + \mathbf{b})$ is convex for any appropriately sized $\mathbf{A}$ and $\mathbf{b}$.
5. If f and g are convex, then $h(\mathbf{x}) \equiv \max\{f(\mathbf{x}); g(\mathbf{x})\}$ is convex.

Some examples

Functions that are convex but not strictly convex:

- $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + \alpha$ for any $\mathbf{w} \in \mathbb{R}^d, \alpha \in \mathbb{R}$. Such a function is called an **affine function**. Note that linear functions and constant functions are special cases of affine functions.
- $f(\mathbf{x}) = \|\mathbf{x}\|_1$.

Functions that are strictly but not strongly convex:

- $f(x) = x^4$.
- $f(x) = \exp(x)$.
- $f(x) = -\log x$.

Functions that are strongly convex:

- $f(\mathbf{x}) = \|\mathbf{x}\|_2^2$

Convexity and existence of minima

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Proposition

Let $\mathcal{X}$ be a convex set. If f is convex, then any local minimum of f in $\mathcal{X}$ is also a global minimum.

Proof

Suppose f is a convex function, and let $\mathbf{x}^*$ be a local minimum of f in $\mathcal{X}$. Then for some neighborhood $N(\mathbf{x}^*) \subset \mathcal{X}$, we have $f(\mathbf{x}) \geq f(\mathbf{x}^*)$, for all $\mathbf{x} \in N(\mathbf{x}^*)$.

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Suppose that there exists $\tilde{\mathbf{x}} \in \mathcal{X}$ such that $f(\tilde{\mathbf{x}}) < f(\mathbf{x}^*)$.
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Consider the line segment $\mathbf{x}(t) = t\,\mathbf{x}^* + (1-t)\tilde{\mathbf{x}}$, $t \in (0,1)$.
Note that $\mathbf{x}(t) \in \mathcal{X}$ by the convexity of $\mathcal{X}$. Then by the convexity of f,

$$f(\mathbf{x}(t)) \leq tf(\mathbf{x}^*) + (1-t)f(\tilde{\mathbf{x}}) < tf(\mathbf{x}^*) + (1-t)f(\mathbf{x}^*) = f(\mathbf{x}^*)$$

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This is absurd, so it follows that $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}$, thus $\mathbf{x}^*$ is a global minimum of f in $\mathcal{X}$.

Proposition

Let $\mathcal{X}$ be a convex set. If f is strictly convex, then there exists at most one local minimum of f in $\mathcal{X}$. Consequently, if it exists it is the unique global minimum of f in $\mathcal{X}$.