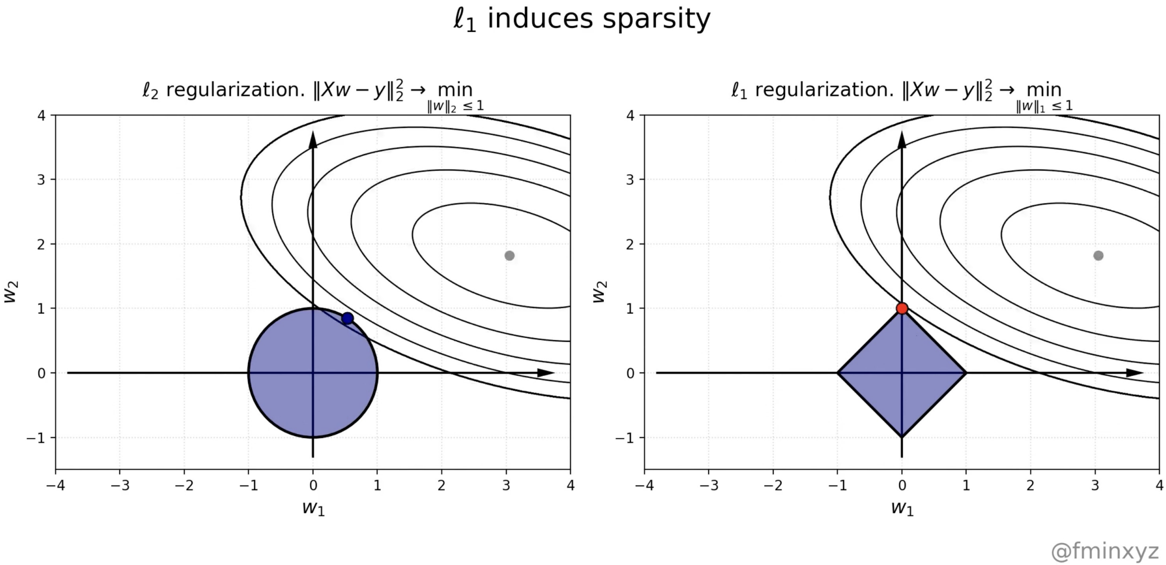
Subgradient. Optimality conditions

Daniil Merkulov

Optimization methods. MIPT

Subgradient and Subdifferential

ℓ_1-regularized linear least squares



Norms are not smooth

$$
\min_{x \in \mathbb{R}^n} f(x),
$$

A classical convex optimization problem is considered. We assume that $f(x)$ is a convex function, but now we do not require smoothness.

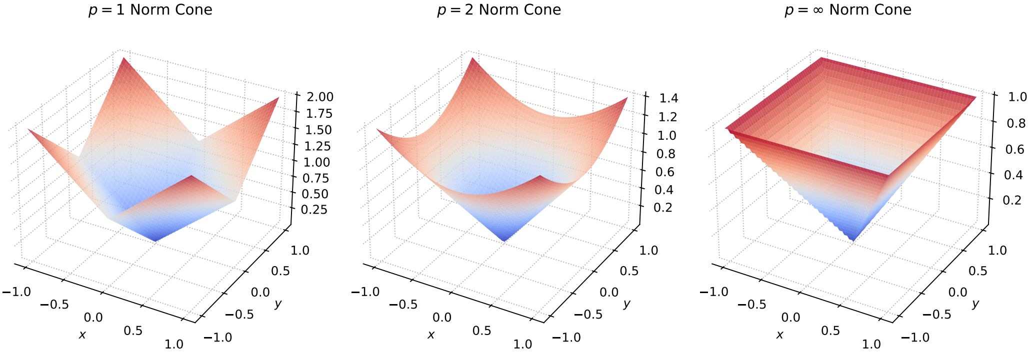


Figure 1: Norm cones for different p - norms are non-smooth

Convex function linear lower bound

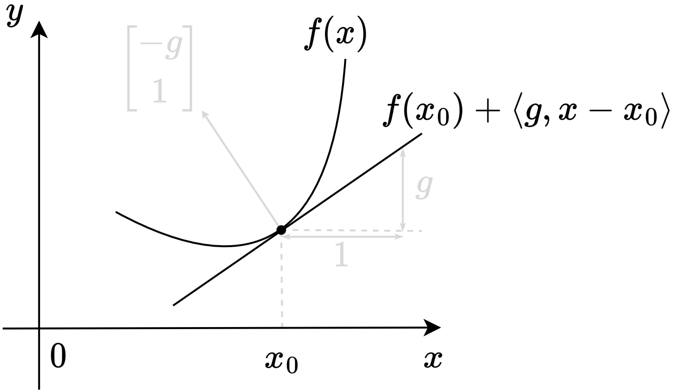


Figure 2: Taylor linear approximation serves as a global lower bound for a convex function

An important property of a continuous convex function $f(x)$ is that at any chosen point x_0 for all $x \in \text{dom } f$ the inequality holds:

$$f(x) \geq f(x_0) + \langle g, x - x_0 \rangle$$

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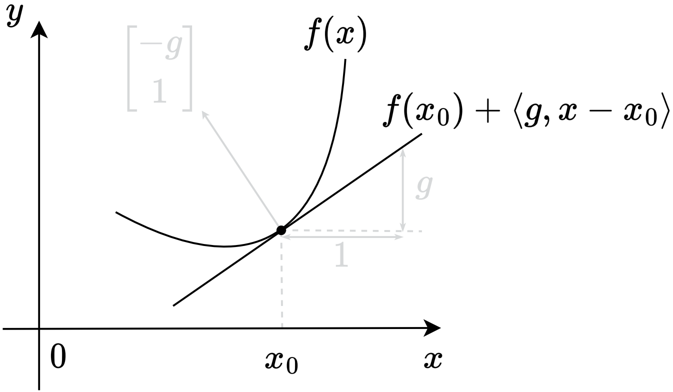

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for some vector g, i.e., the tangent to the graph of the function is the *global* estimate from below for the function.

- If $f(x)$ is differentiable, then $g = \nabla f(x_0)$

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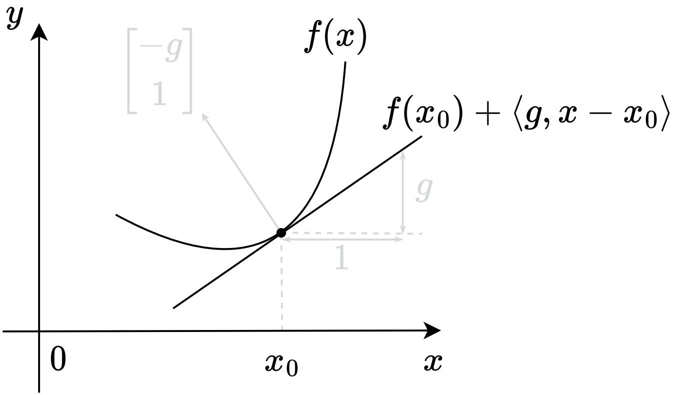

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- Not all continuous convex functions are differentiable.

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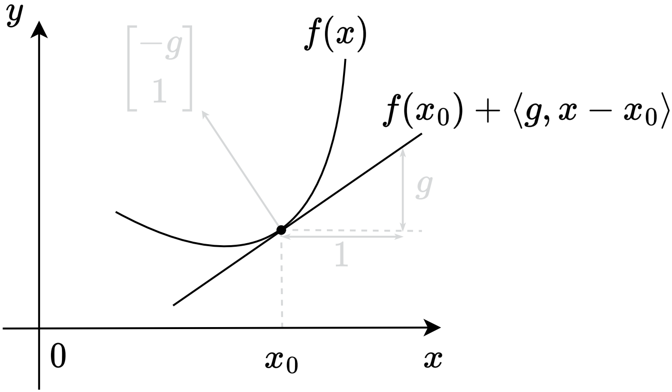

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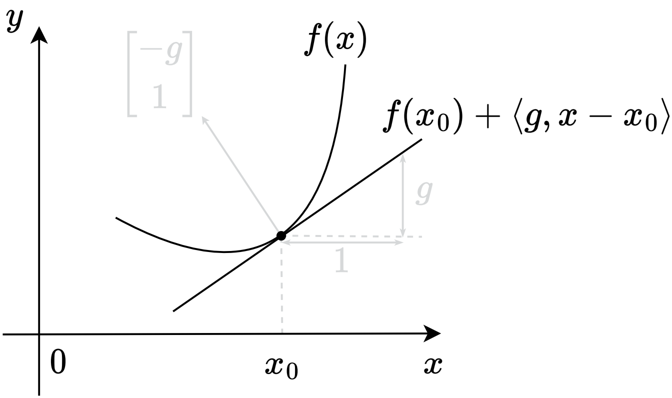

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We wouldn't want to lose such a nice property.

Subgradient and subdifferential

A vector g is called the **subgradient** of a function $f(x) : S \to \mathbb{R}$ at a point x_0 if $\forall x \in S$:

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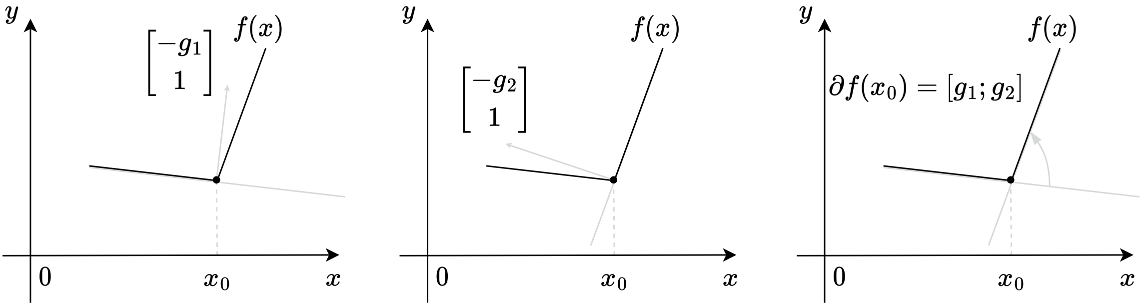

Figure 3: Subdifferential is a set of all possible subgradients

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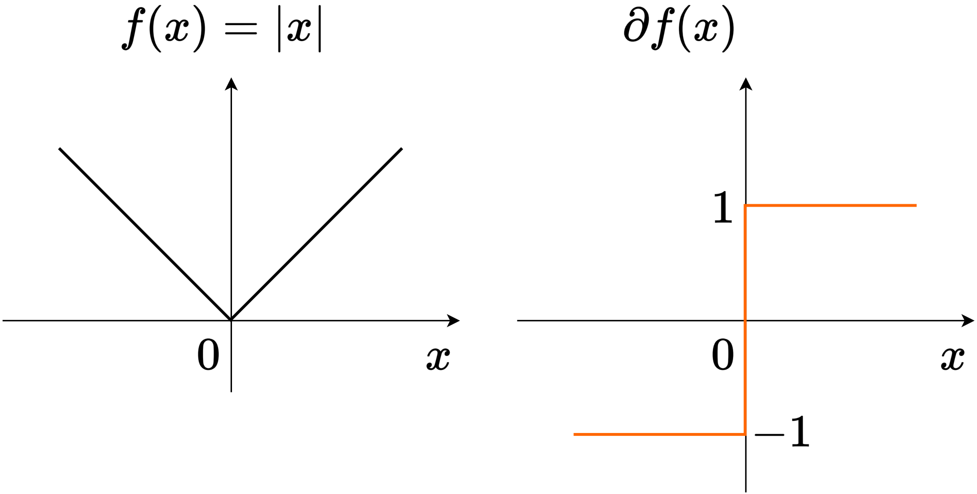

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Subdifferential of a differentiable function

Let $f : S \to \mathbb{R}$ be a function defined on the set S in a Euclidean space $\mathbb{R}^n$. If $x_0 \in \mathbf{ri}(S)$ and f is differentiable at x_0, then either $\partial f(x_0) = \emptyset$ or $\partial f(x_0) = \{\nabla f(x_0)\}$. Moreover, if the function f is convex, the first scenario is impossible.

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Proof

1. Assume, that $s \in \partial f(x_0)$ for some $s \in \mathbb{R}^n$ distinct from $\nabla f(x_0)$. Let $v \in \mathbb{R}^n$ be a unit vector. Because x_0 is an interior point of S, there exists $\delta > 0$ such that $x_0 + tv \in S$ for all $0 < t < \delta$. By the definition of the subgradient, we have

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f(x_0 + tv) \geq f(x_0) + t\langle s, v\rangle
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which implies:

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for all $0 < t < \delta$. Taking the limit as t approaches 0 and using the definition of the gradient, we get:

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\langle \nabla f(x_0), v\rangle = \lim_{t \to 0; 0 < t < \delta} \frac{f(x_0 + tv) - f(x_0)}{t} \geq \langle s, v\rangle
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2. From this, $\langle s - \nabla f(x_0), v\rangle \geq 0$. Due to the arbitrariness of v, one can set

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v = -\frac{s - \nabla f(x_0)}{\|s - \nabla f(x_0)\|},
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leading to $s = \nabla f(x_0)$.

3. Furthermore, if the function f is convex, then according to the differential condition of convexity $f(x) \geq f(x_0) + \langle \nabla f(x_0), x - x_0\rangle$ for all $x \in S$. But by definition, this means $\nabla f(x_0) \in \partial f(x_0)$.

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Is it correct, that if the function has a subdifferential at some point, the function is convex?

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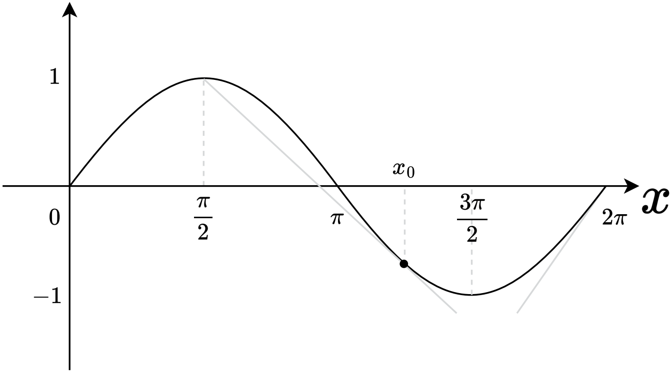
Find $\partial f(x)$, if $f(x) = \sin x, x \in [\pi/2; 2\pi]$



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Convexity follows from subdifferentiability at any point. A natural question to ask is whether the converse is true: is every convex function subdifferentiable? It turns out that, generally speaking, the answer to this question is negative.

Let $f : [0, \infty) \to \mathbb{R}$ be the function defined by $f(x) := -\sqrt{x}$. Then, $\partial f(0) = \emptyset$.

Assume, that $s \in \partial f(0)$ for some $s \in \mathbb{R}$. Then, by definition, we must have $sx \leq -\sqrt{x}$ for all $x \geq 0$. From this, we can deduce $s \leq -\sqrt{1}$ for all $x > 0$. Taking the limit as x approaches 0 from the right, we get $s \leq -\infty$, which is impossible.

Subdifferential calculus

Moreau - Rockafellar theorem (subdifferential of a linear combination)

Let $f_i(x)$ be convex functions on convex sets $S_i,\ i = \overline{1,n}$. Then if $\bigcap\limits_{i=1}^n \mathbf{ri}(S_i) \neq \emptyset$ then the function $f(x) = \sum\limits_{i=1}^n a_i f_i(x),\ a_i > 0$ has a subdifferential $\partial_S f(x)$ on the set $S = \bigcap\limits_{i=1}^n S_i$ and

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Dubovitsky - Milutin theorem (subdifferential of a point-wise maximum)

Let $f_i(x)$ be convex functions on the open convex set $S \subseteq \mathbb{R}^n,\ x_0 \in S$, and the pointwise maximum is defined as $f(x) = \max\limits_i f_i(x)$. Then:

$$
\partial_S f(x_0) = \mathbf{conv}\left\{ \bigcup_{i \in I(x_0)} \partial_S f_i(x_0) \right\}, \quad I(x) = \{i \in [1
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- $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$.

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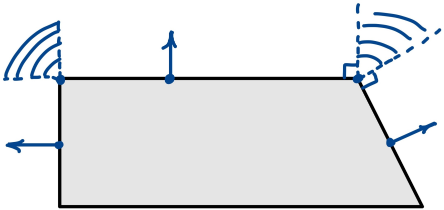
- $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$.
- Let $f : E \to \mathbb{R}$ be a convex function and $g : \mathbb{R} \to \mathbb{R}$ be a nondecreasing convex function. Let $x \in E$, and suppose that g is differentiable at the point $f(x)$. Let $h = g \circ f$. Then $\partial h(x) = g'(f(x))\partial f(x)$.

Connection to convex geometry

Convex set $S \subseteq \mathbb{R}^n$, consider indicator function $I_S : \mathbb{R}^n \to \mathbb{R}$,

$$I_S(x) = I\{x \in S\} = \begin{cases} 0 & \text{if } x \in S \\ \infty & \text{if } x \notin S \end{cases}$$



For $x \in S$, $\partial I_S(x) = \mathcal{N}_S(x)$, the **normal cone** of S at x is, recall

$$\mathcal{N}_S(x) = \{g \in \mathbb{R}^n : g^T x \geq g^T y \text{ for any } y \in S\}$$

Why? By definition of subgradient g,

$$I_S(y) \geq I_S(x) + g^T(y - x) \quad \text{for all } y$$

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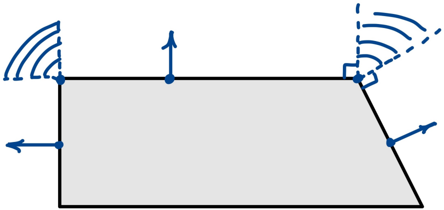

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- For $y \notin S$, $I_S(y) = \infty$
- For $y \in S$, this means $0 \geq g^T(y - x)$

Optimality Condition

For any f (convex or not),

$$f(x^\star) = \min_x f(x) \quad \Longleftrightarrow \quad 0 \in \partial f(x^\star)$$

That is, $x^\star$ is a minimizer if and only if 0 is a subgradient of f at $x^\star$. This is called the **subgradient optimality condition**.

Why? Easy: $g = 0$ being a subgradient means that for all y

$$f(y) \geq f(x^\star) + 0^T(y - x^\star) = f(x^\star)$$

Note the implication for a convex and differentiable function f, with

$$\partial f(x) = \{\nabla f(x)\}$$

Derivation of first-order optimality

Example of the power of subgradients: we can use what we have learned so far to derive the **first-order optimality condition**. Recall

$$\min_x f(x) \text{ subject to } x \in S$$

is solved at x, for f convex and differentiable, if and only if

$$\nabla f(x)^T(y - x) \geq 0 \quad \text{for all } y \in S$$

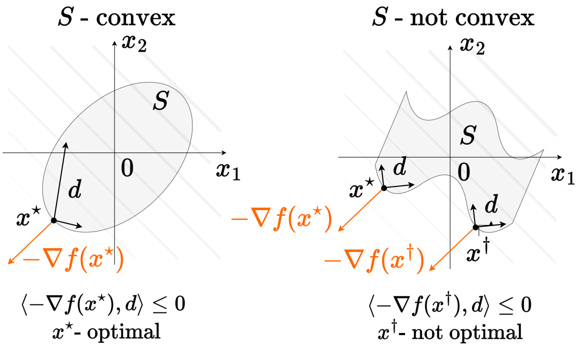
Intuitively: this says that the gradient increases as we move away from x. How to prove it? First, recast the problem as

$$\min_x f(x) + I_S(x)$$

Now apply subgradient optimality:

$$0 \in \partial(f(x) + I_S(x))$$

$$f(x) = x_1 + x_2 \to \min_{x_1, x_2 \in \mathbb{R}^2}$$



Derivation of first-order optimality

Observe

$$0 \in \partial(f(x) + I_S(x))$$

$$\Leftrightarrow 0 \in \{\nabla f(x)\} + \mathcal{N}_S(x)$$

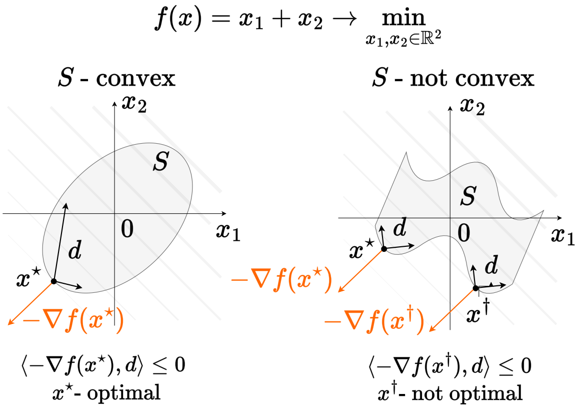
$$\Leftrightarrow -\nabla f(x) \in \mathcal{N}_S(x)$$

$$\Leftrightarrow -\nabla f(x)^T x \geq -\nabla f(x)^T y \text{ for all } y \in S$$

$$\Leftrightarrow \nabla f(x)^T (y - x) \geq 0 \text{ for all } y \in S$$

as desired.

Note: the condition $0 \in \partial f(x) + \mathcal{N}_S(x)$ is a **fully general condition** for optimality in convex problems. But it's not always easy to work with (KKT conditions, later, are easier).



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$$\partial f_1(x) = \begin{cases} -1, & x < 1 \\ [-1;1], & x = 1 \\ 1, & x > 1 \end{cases} \qquad \partial f_2(x) = \begin{cases} -1, & x < -1 \\ [-1;1], & x = -1 \\ 1, & x > -1 \end{cases}$$

So

$$\partial f(x) = \begin{cases} -2, & x < -1 \\ [-2;0], & x = -1 \\ 0, & -1 < x < 1 \\ [0;2], & x = 1 \\ 2, & x > 1 \end{cases}$$

Example 2

Find $\partial f(x)$ if $f(x) = [\max(0, f_0(x))]^q$. Here, $f_0(x)$ is a convex function on an open convex set S, and $q \geq 1$.

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According to the composition theorem (the function $\varphi(x) = x^q$ is differentiable) and $g(x) = \max(0, f_0(x))$, we have:

$$\partial f(x) = q(g(x))^{q-1}\partial g(x)$$

By the theorem on the pointwise maximum:

$$\partial g(x) = \begin{cases} \partial f_0(x), & f_0(x) > 0, \\ \{0\}, & f_0(x) < 0, \\ \{a \mid a = \lambda a',\ 0 \leq \lambda \leq 1,\ a' \in \partial f_0(x)\}, & f_0(x) = 0 \end{cases}$$

Example 3. Subdifferential of the Norm

Let V be a finite-dimensional Euclidean space, and $x_0 \in V$. Let $\|\cdot\|$ be an arbitrary norm in V (not necessarily induced by the scalar product), and let $\|\cdot\|_*$ be the corresponding conjugate norm. Then,

$$\partial\|\cdot\|(x_0) = \begin{cases} B_{\|\cdot\|_*}(0,1), & \text{if } x_0 = 0, \\ \{s \in V : \|s\|_* \leq 1; \langle s, x_0\rangle = \|x_0\|\} = \{s \in V : \|s\|_* = 1; \langle s, x_0\rangle = \|x_0\|\}, & \text{otherwise.} \end{cases}$$

Where $B_{\|\cdot\|_*}(0,1)$ is the closed unit ball centered at zero with respect to the conjugate norm. In other words, a vector $s \in V$ with $\|s\|_* = 1$ is a subgradient of the norm $\|\cdot\|$ at point $x_0 \neq 0$ if and only if the Hölder's inequality $\langle s, x_0\rangle \leq \|x_0\|$ becomes an equality.

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or equivalently,

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It is important to note that the expression on the left side is the supremum from the definition of the Fenchel conjugate function for the norm, which is known to be

$$\sup_{x \in V}\{\langle s, x\rangle - \|x\|\} = \begin{cases} 0, & \text{if } \|s\|_* \leq 1, \\ +\infty, & \text{otherwise.} \end{cases}$$

Thus, equation is equivalent to $\|s\|_* \leq 1$ and $\langle s, x_0\rangle = \|x_0\|$.

Example 3. Subdifferential of the Norm

Consequently, it remains to note that for $x_0 \neq 0$, the inequality $\|s\|_* \leq 1$ must become an equality since, when $\|s\|_* < 1$, Hölder's inequality implies $\langle s, x_0 \rangle \leq \|s\|_* \|x_0\| < \|x_0\|$.

The conjugate norm in Example above does not appear by chance. It turns out that, in a completely similar manner for an arbitrary function f (not just for the norm), its subdifferential can be described in terms of the dual object — the Fenchel conjugate function.

Optimality conditions

Background

$$f(x) \to \min_{x \in S}$$

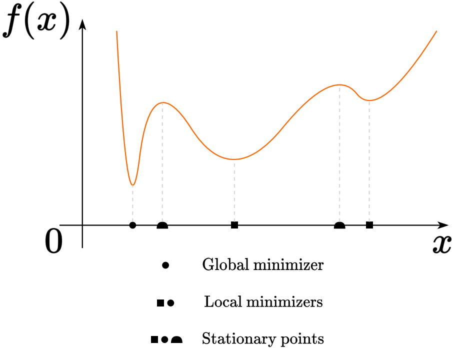

Figure 5: Illustration of different stationary (critical) points

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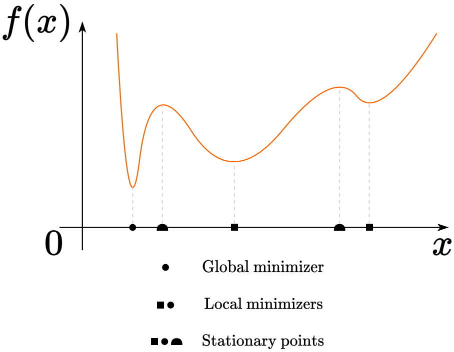

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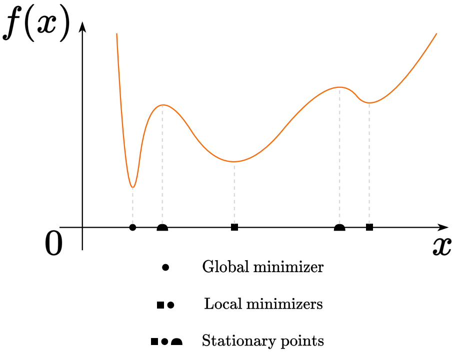

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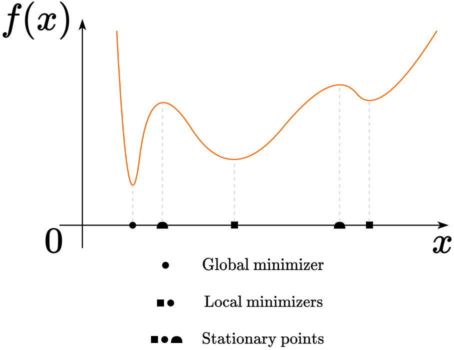

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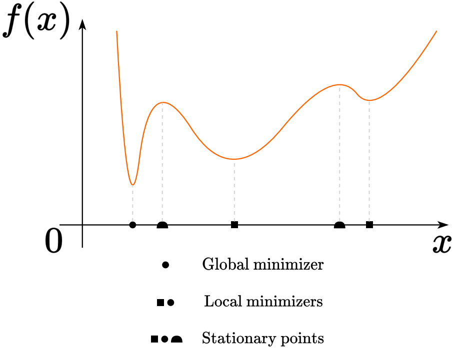

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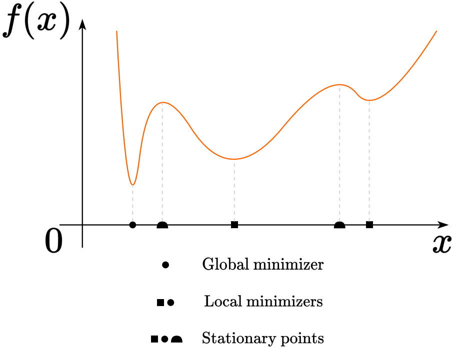

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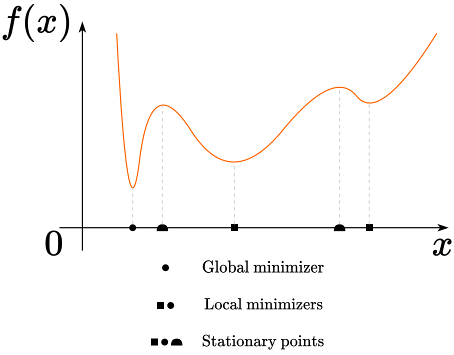

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- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

Extreme value (Weierstrass) theorem

Theorem

Let $S \subset \mathbb{R}^n$ be a compact set and $f(x)$ a continuous function on S. So, the point of the global minimum of the function $f(x)$ on S exists.

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Figure 6: A lot of practical problems are theoretically solvable

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Figure 6: A lot of practical problems are theoretically solvable

Taylor's Theorem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and that $p \in \mathbb{R}^n$. Then we have:

$$f(x+p) = f(x) + \nabla f(x+tp)^T p \quad \text{for some } t \in (0,1)$$

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Moreover, if f is twice continuously differentiable, we have:

$$\nabla f(x+p) = \nabla f(x) + \int_0^1 \nabla^2 f(x+tp)p \, dt$$

$$f(x+p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x+tp) p$$

for some $t \in (0,1)$.

Unconstrained optimization

Necessary Conditions

First-Order Necessary Conditions

If x^* is a local minimizer and f is continuously differentiable in an open neighborhood, then

$$\nabla f(x^*) = 0$$

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Therefore, $f(x^* + \bar{t}p) < f(x^*)$ for all $\bar{t} \in (0, T]$. We have found a direction from x^* along which f decreases, so x^* is not a local minimizer, leading to a contradiction.

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Second-Order Sufficient Conditions

Suppose that $\nabla^2 f$ is continuous in an open neighborhood of x^* and that

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where $z = x^* + tp$ for some $t \in (0, 1)$. Since $z \in B$, we have $p^T \nabla^2 f(z) p > 0$, and therefore $f(x^* + p) > f(x^*)$, giving the result.

Peano counterexample

Note, that if $\nabla f(x^*) = 0, \nabla^2 f(x^*) \succeq 0$, i.e. the hessian is positive *semidefinite*, we cannot be sure if x^* is a local minimum.

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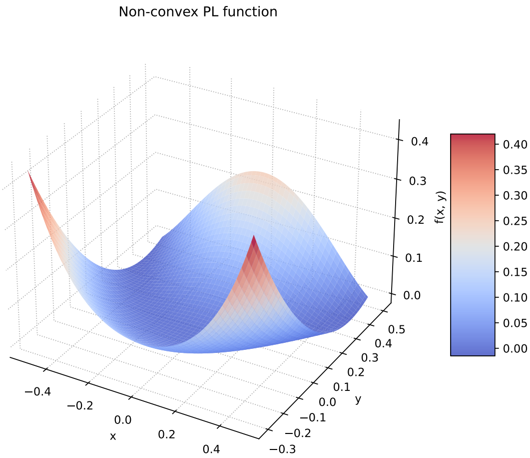

Constrained optimization

General first-order local optimality condition

Direction $d \in \mathbb{R}^n$ is a feasible direction at $x^* \in S \subseteq \mathbb{R}^n$ if small steps along d do not take us outside of S.

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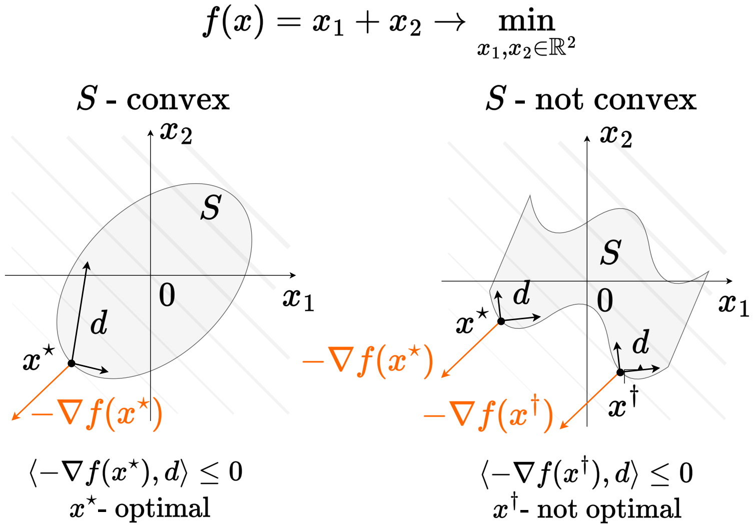

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Convex case

It should be mentioned, that in the **convex** case (i.e., $f(x)$ is convex) necessary condition becomes sufficient.

One more important result for the convex unconstrained case sounds as follows. If $f(x) : S \to \mathbb{R}$ - convex function defined on the convex set S, then:

- Any local minima is the global one.
- The set of the local minimizers S^* is convex.
- If $f(x)$ - strictly or strongly convex function, then S^* contains only one single point $S^* = \{x^*\}$.

Optimization with equality constraints

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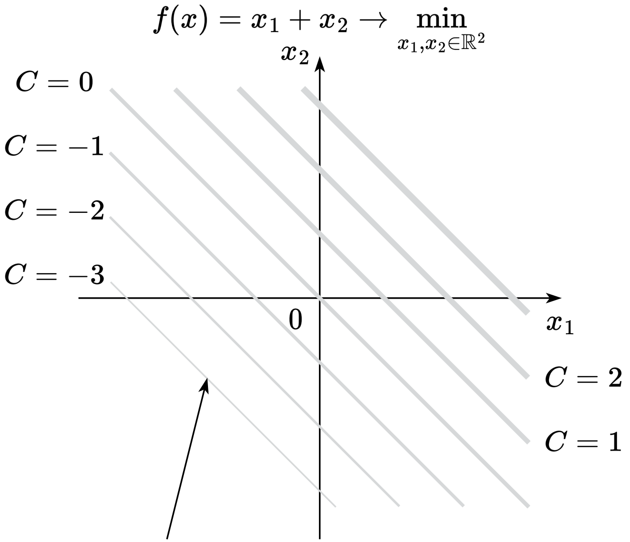
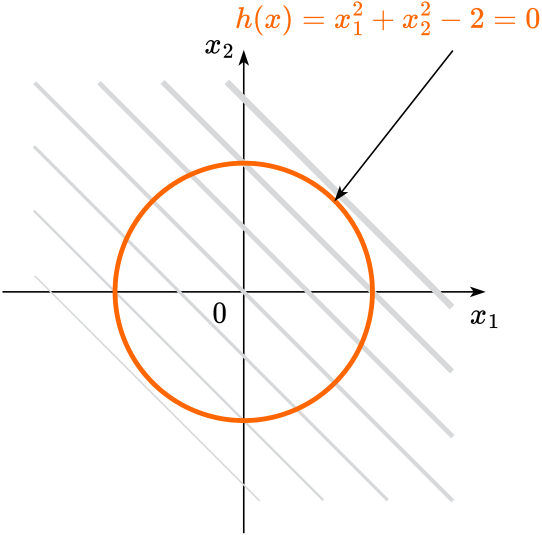
We will try to illustrate an approach to solve this problem through the simple example with $f(x) = x_1 + x_2$ and $h(x) = x_1^2 + x_2^2 - 2$.

Optimization with equality constraints



Contour lines of $f(x) = x_1 + x_2 = C$

Optimization with equality constraints



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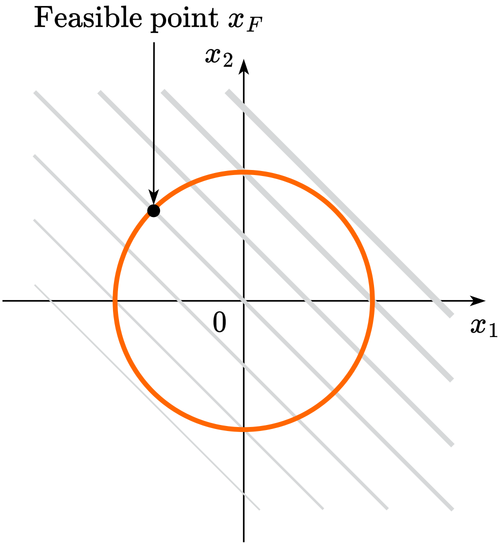

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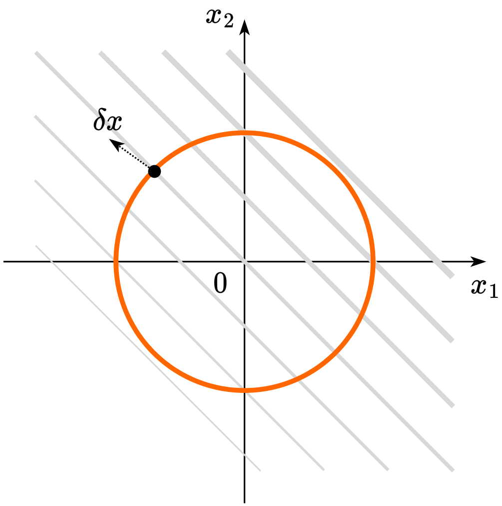

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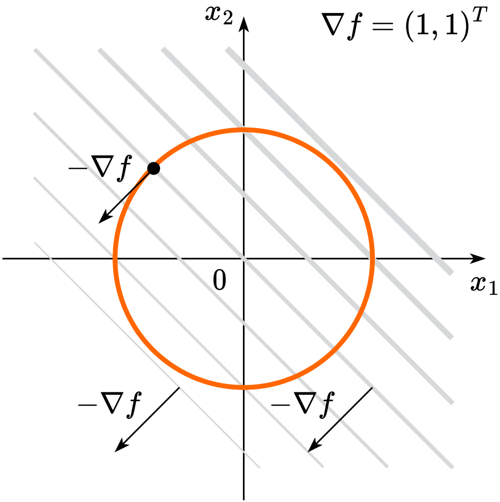

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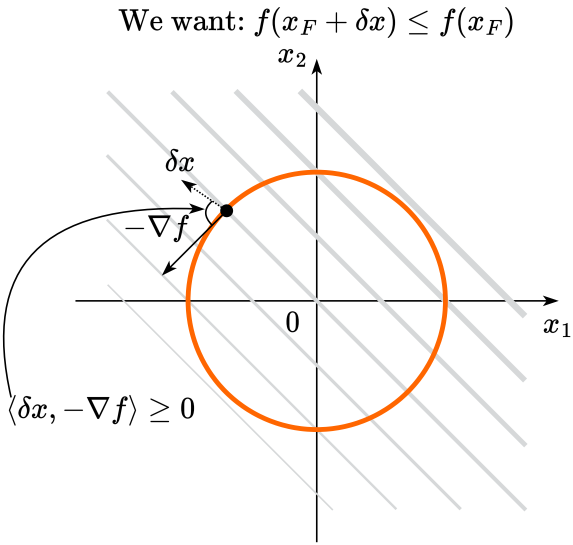

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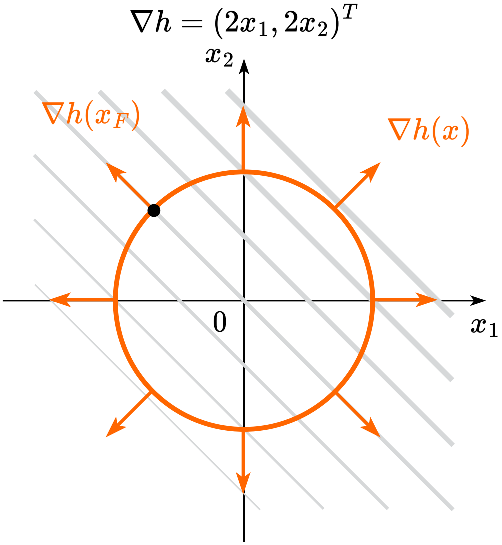

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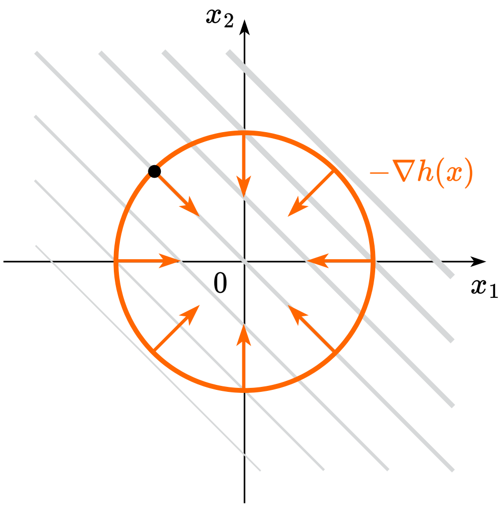

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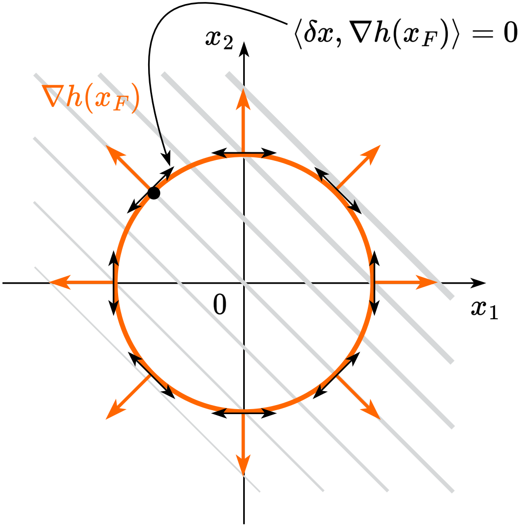

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Then we came to the point of the budget set, moving from which it will not be possible to reduce our function. This is the local minimum in the constrained problem :)

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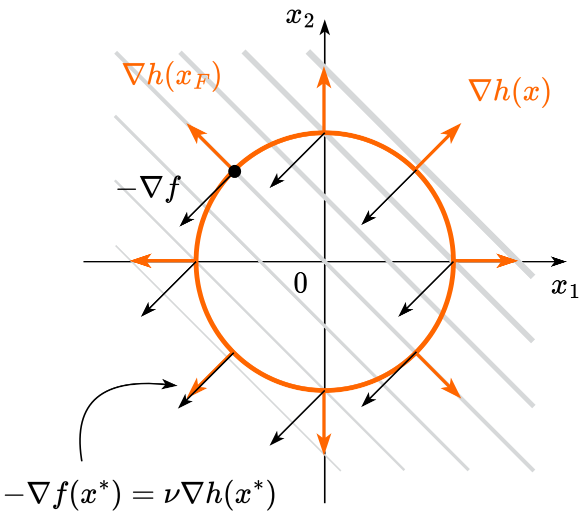

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Equality constrained problem

$$
\begin{split}
& f(x) \to \min\limits_{x \in \mathbb{R}^n} \\
\text{s.t. } & h_i(x) = 0, \; i = 1, \ldots, p
\end{split} \tag{ECP}
$$

$$
L(x, \nu) = f(x) + \sum\limits_{i=1}^p \nu_i h_i(x) = f(x) + \nu^\top h(x)
$$

Let $f(x)$ and $h_i(x)$ be twice differentiable at the point x^* and continuously differentiable in some neighborhood x^*. The local minimum conditions for $x \in \mathbb{R}^n, \nu \in \mathbb{R}^p$ are written as

ECP: Necessary conditions

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ECP: Sufficient conditions

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Linear Least Squares

Example

Pose the optimization problem and solve them for linear system $Ax = b, A \in \mathbb{R}^{m \times n}$ for three cases (assuming the matrix is full rank):

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