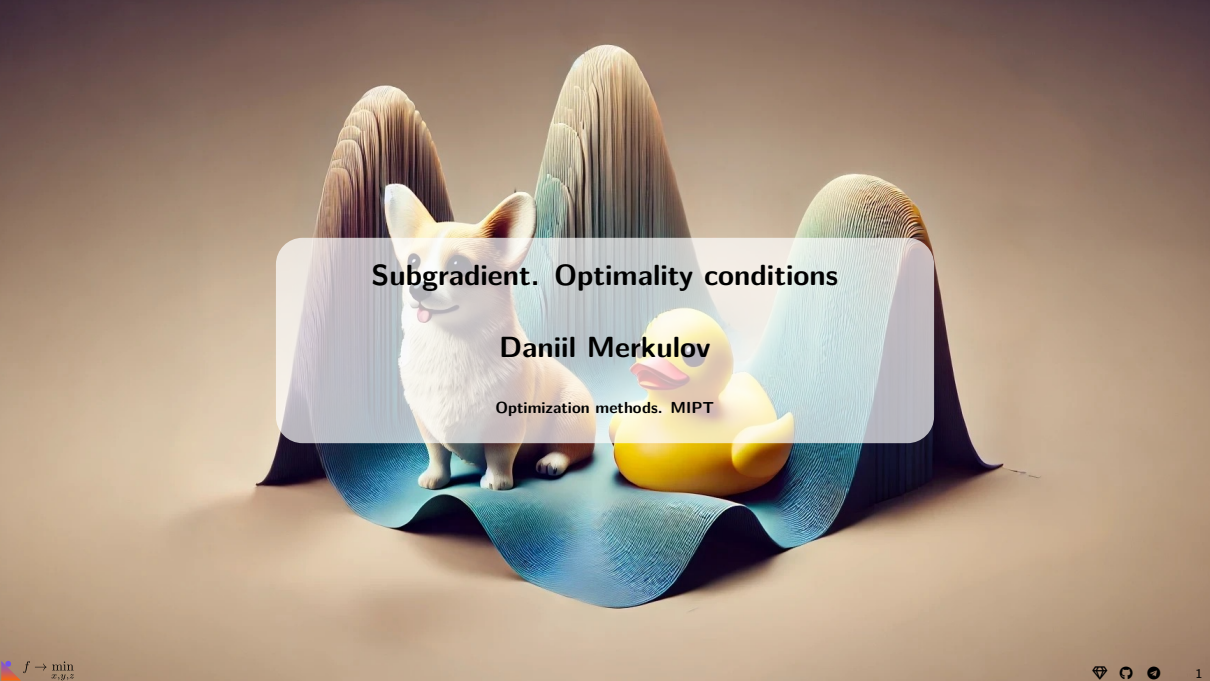


Subgradient. Optimality conditions

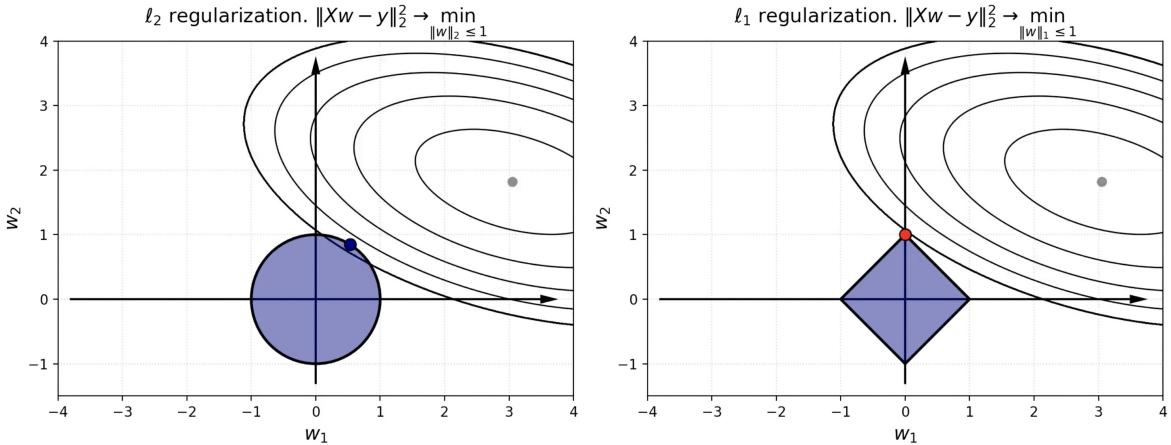
Daniil Merkulov

Optimization methods. MIPT

Subgradient and Subdifferential

ℓ_1-regularized linear least squares

ℓ_1 induces sparsity



@fminxyz

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.

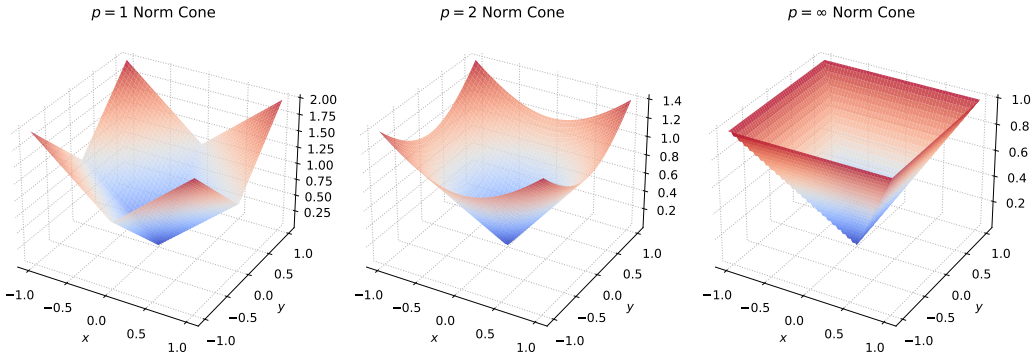


Figure 1: Norm cones for different p - norms are non-smooth

Convex function linear lower bound

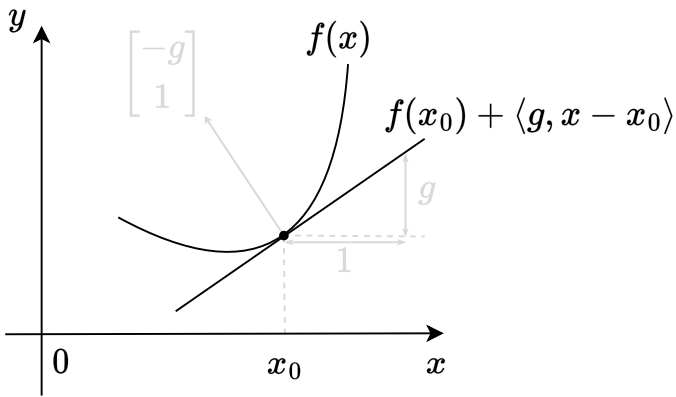


Figure 2: Taylor linear approximation serves as a global lower bound for a convex function

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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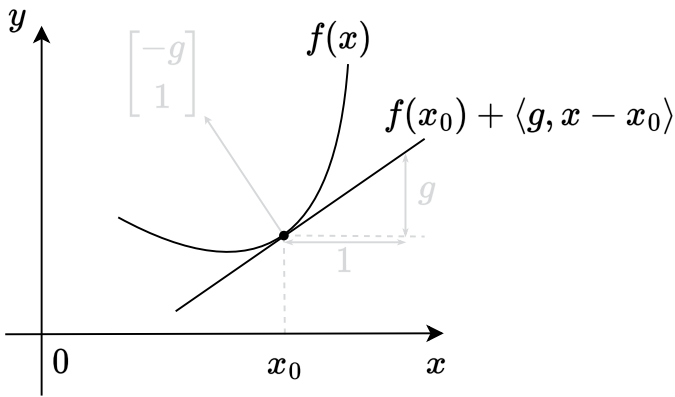

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for some vector g, i.e., the tangent to the graph of the function is the *global* estimate from below for the function.

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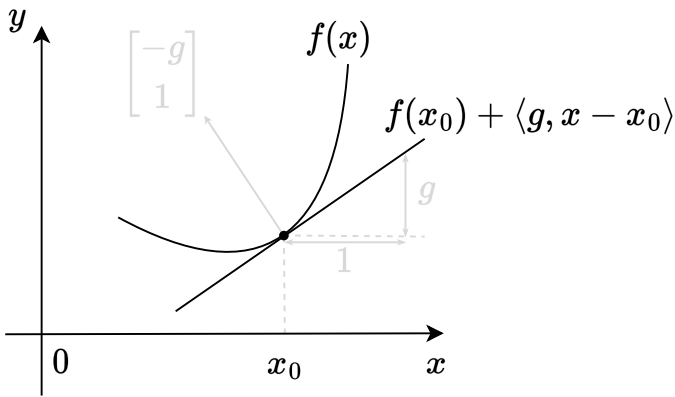

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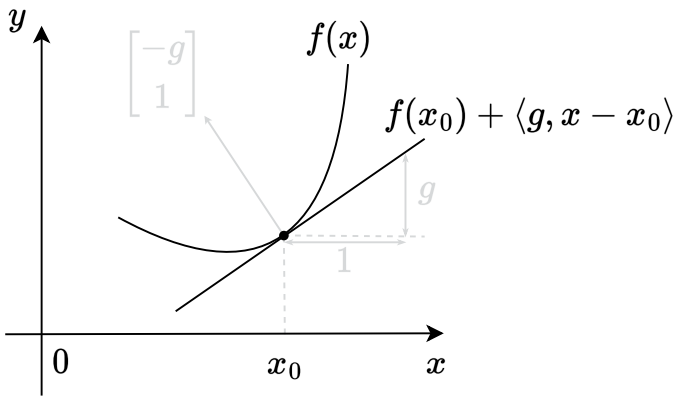

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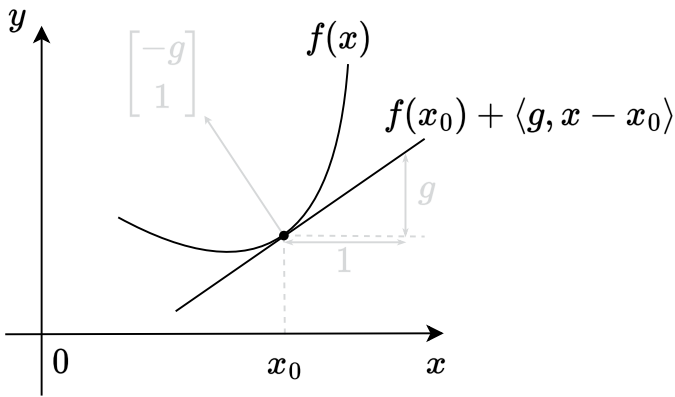

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We wouldn't want to lose such a nice property.

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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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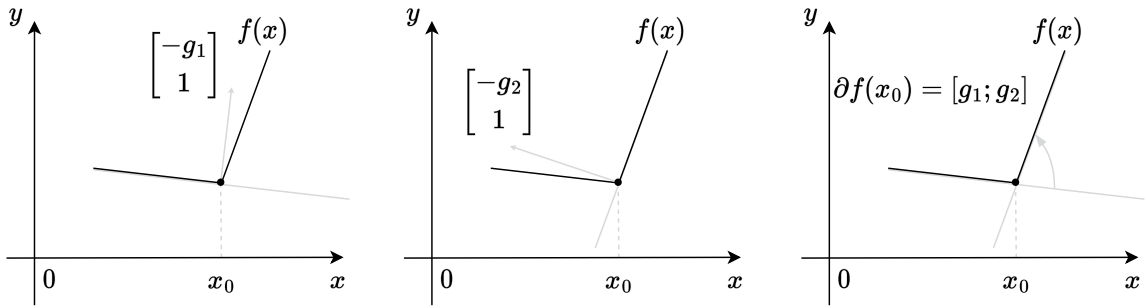

Figure 3: Subdifferential is a set of all possible subgradients

Subgradient and subdifferential

Find $\partial f(x)$, if $f(x) = |x|$

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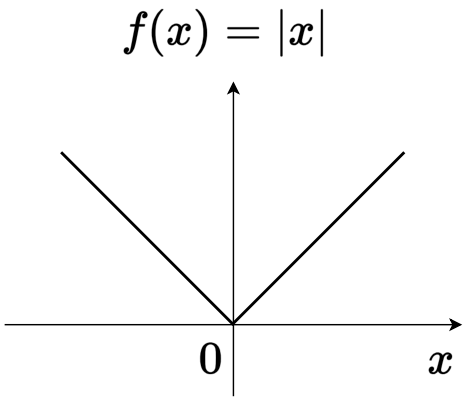

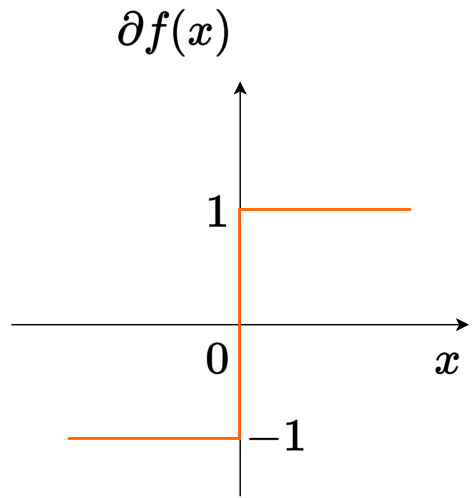

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Subdifferential of a differentiable function

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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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$$\langle \nabla f(x_0), v\rangle = \lim_{t \to 0; 0 < t < \delta} \frac{f(x_0 + tv) - f(x_0)}{t} \geq \langle s, v\rangle$$

2. From this, $\langle s - \nabla f(x_0), v\rangle \geq 0$. Due to the arbitrariness of v, one can set

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

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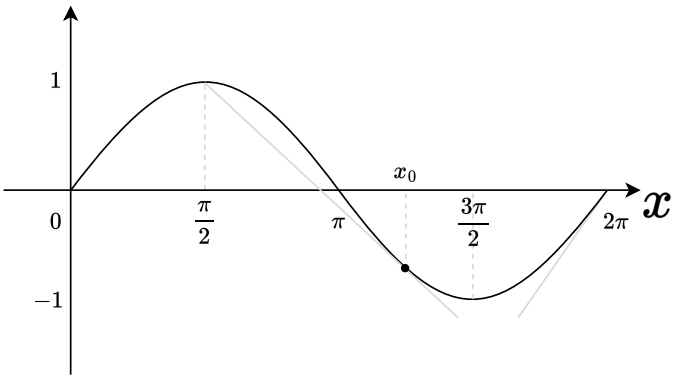
Find $\partial f(x)$, if $f(x) = \sin x, x \in [\pi/2; 2\pi]$



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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 $\bigcap_{i=1}^{n} \mathbf{ri}(S_i) \neq \emptyset$ then the function $f(x) = \sum_{i=1}^{n} a_i f_i(x),\ a_i > 0$ has a subdifferential $\partial_S f(x)$ on the set $S = \bigcap_{i=1}^{n} S_i$ 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 $x \in \partial f^*(z)$.
- 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 $I_S : \mathbb{R}^n \to \mathbb{R}$,

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

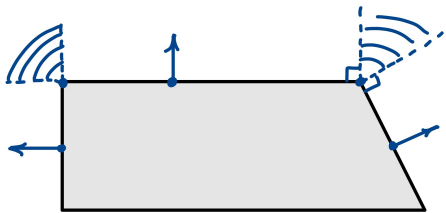
For $x \in S$, $\partial I_S(x) = \mathcal{N}_S(x)$, the **normal cone** of S at x is, recall

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

Why? By definition of subgradient g,

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

- For $y \notin S$, $I_S(y) = \infty$



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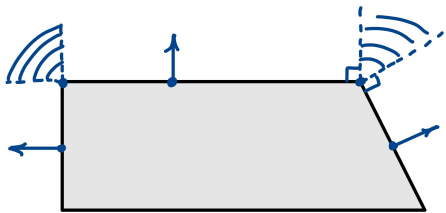
- For $y \in S$, this means $0 \geq g^T(y - x)$



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

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

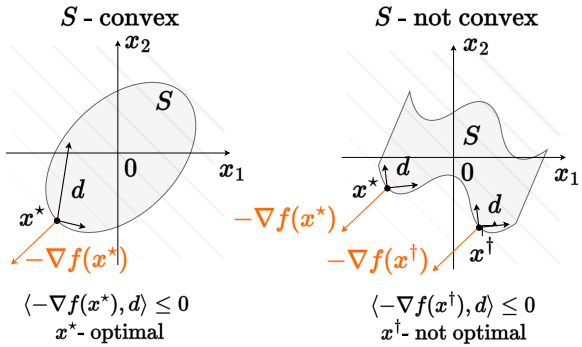
Intuitively: this says that the gradient increases as we move away from x. How to prove it? First, recast the problem as

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

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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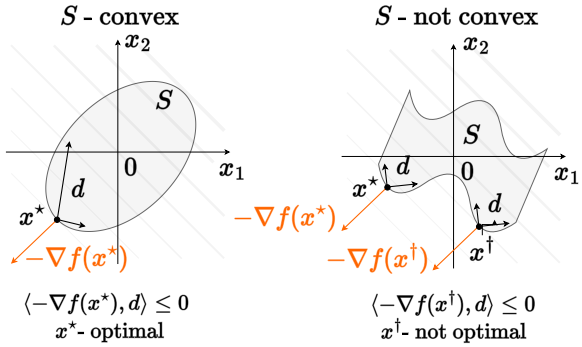

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$$\partial f_1(x) = \begin{cases} -1, & x < 1 \\ [-1;1], & x = 1 \\ 1, & x > 1 \end{cases} \qquad \partial f_2(x) = \begin{cases} -1, & x < -1 \\ [-1;1], & x = -1 \\ 1, & x > -1 \end{cases}$$

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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Let $s \in V$. By definition, $s \in \partial\|\cdot\|(x_0)$ if and only if

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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

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

Thus, equation is equivalent to $\|s\|_* \le 1$ 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

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

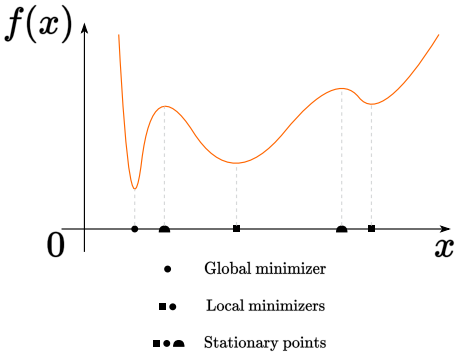

Figure 5: Illustration of different stationary (critical) points

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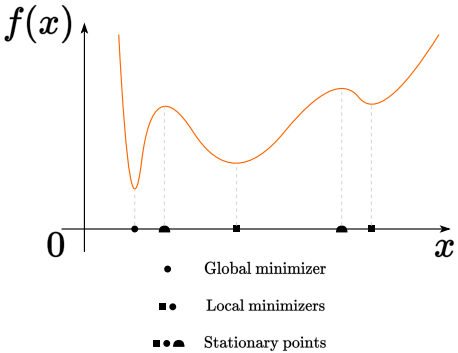

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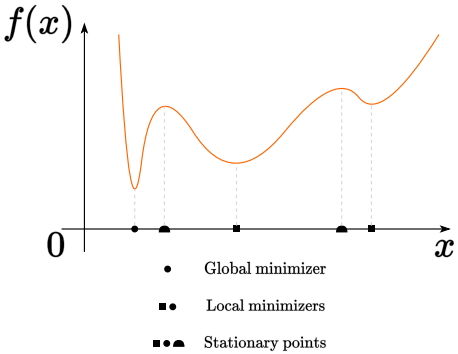

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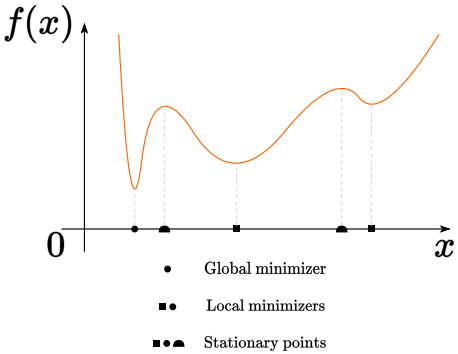

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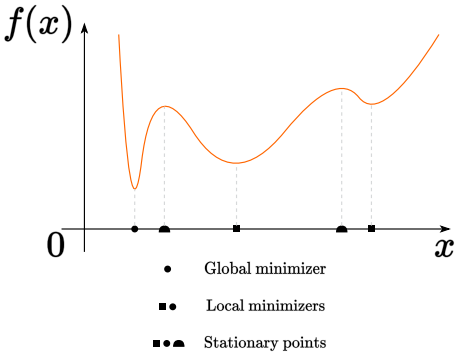

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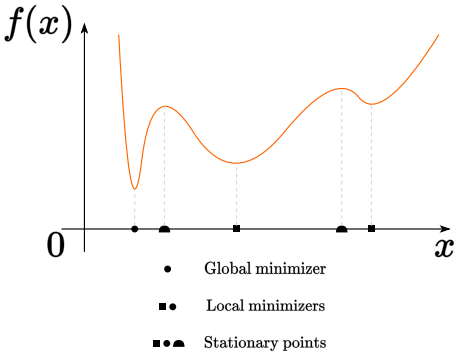

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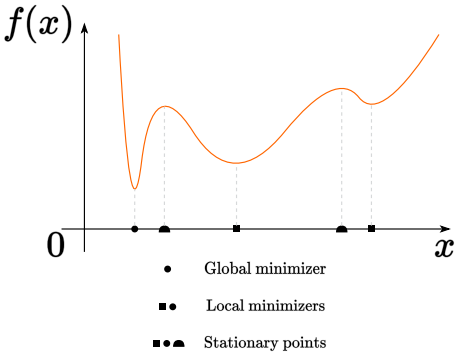

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- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

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

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First-Order Necessary Conditions

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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.

Sufficient Conditions

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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Although the surface does not have a local minimizer at the origin, its intersection with any vertical plane through the origin (a plane with equation $y = mx$ or $x = 0$) is a curve that has a local minimum at the origin. In other words, if a point starts at the origin $(0, 0)$ of the plane, and moves away from the origin along any straight line, the value of $(2x^2 - y)(x^2 - y)$ will increase at the start of the motion. Nevertheless, $(0, 0)$ is not a local minimizer of the function, because moving along a parabola such as $y = \sqrt{2}x^2$ will cause the function value to decrease.

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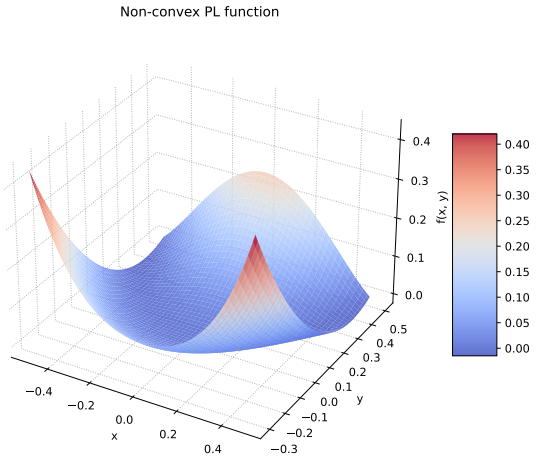

Constrained optimization

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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Consider a set $S \subseteq \mathbb{R}^n$ and a function $f : \mathbb{R}^n \to \mathbb{R}$. Suppose that $x^* \in S$ is a point of local minimum for f over S, and further assume that f is continuously differentiable around x^*.

General first-order local optimality condition

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Consider a set $S \subseteq \mathbb{R}^n$ and a function $f : \mathbb{R}^n \to \mathbb{R}$. Suppose that $x^* \in S$ is a point of local minimum for f over S, and further assume that f is continuously differentiable around x^*.

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

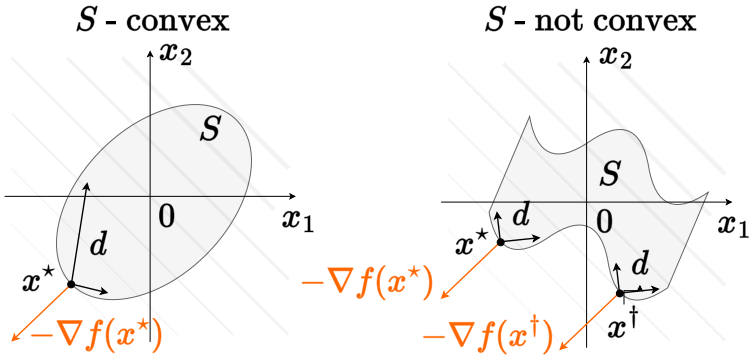

Figure 7: General first order local optimality condition

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

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- 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 $S^* = \{x^*\}$.

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Things are pretty simple and intuitive in unconstrained problems. In this section, we will add one equality constraint, i.e.

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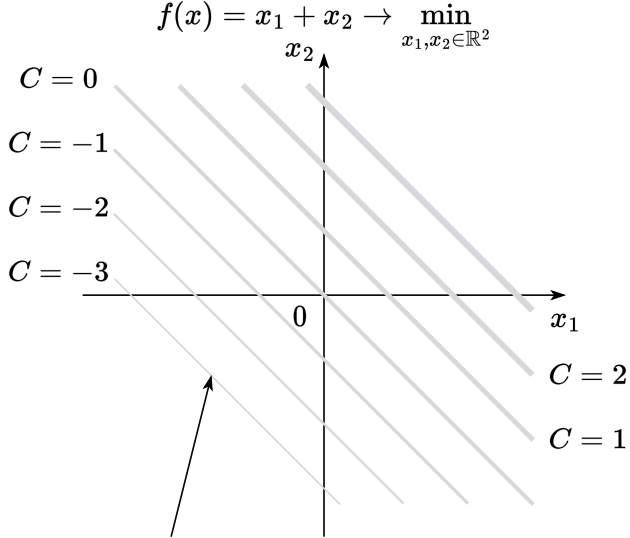
We will try to illustrate an approach to solve this problem through the simple example with $f(x) = x_1 + x_2$ and $h(x) = x_1^2 + x_2^2 - 2$.

Optimization with equality constraints



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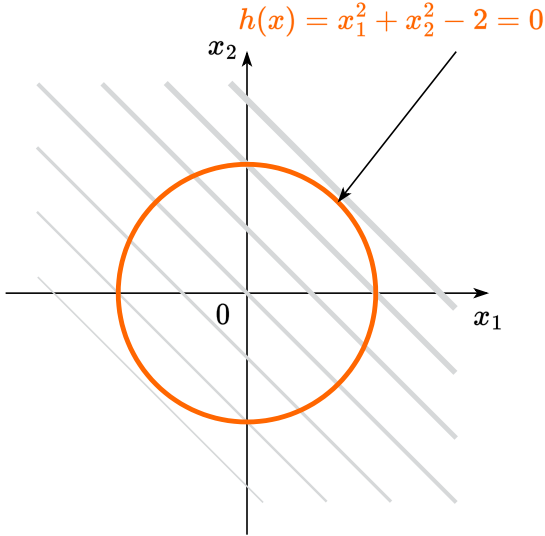

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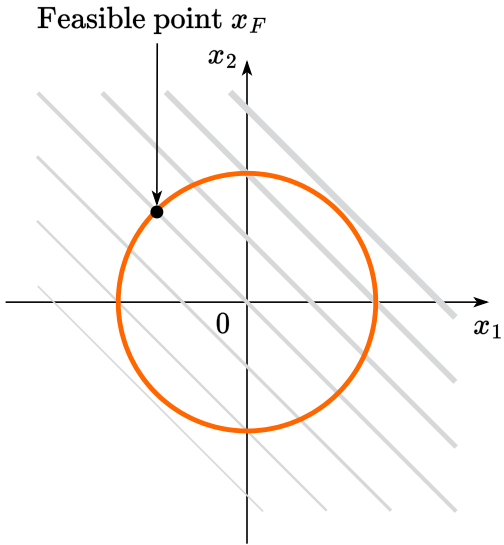

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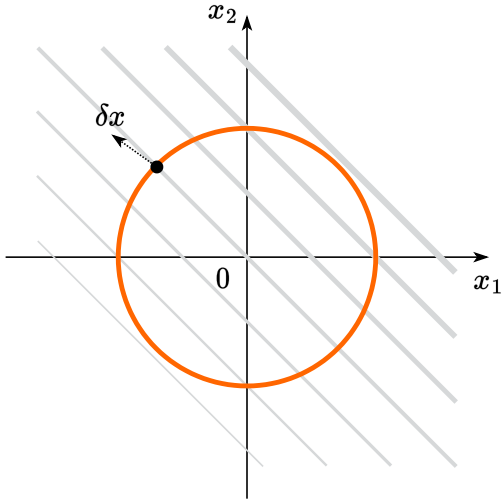

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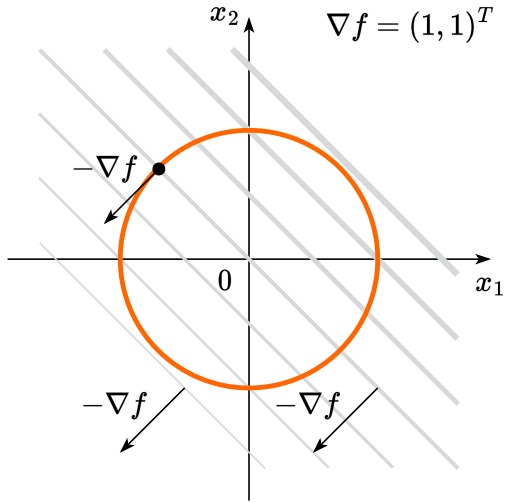

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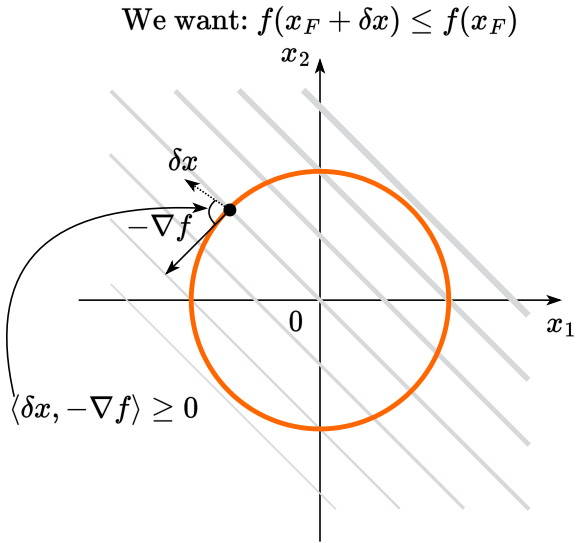

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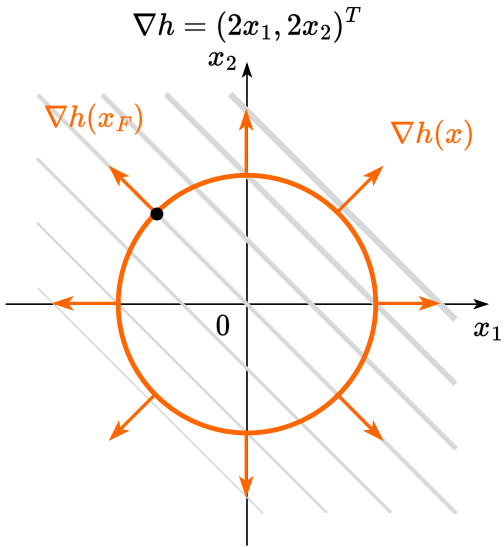

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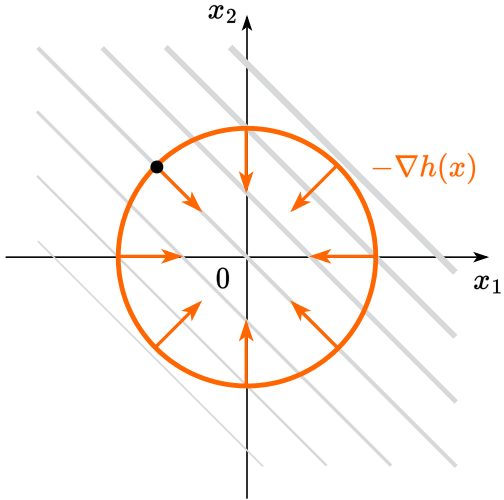

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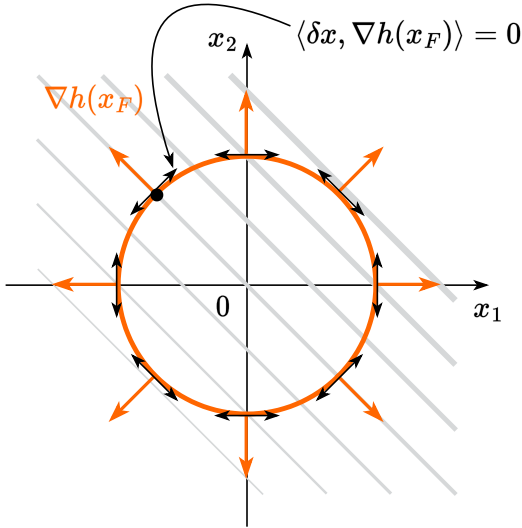

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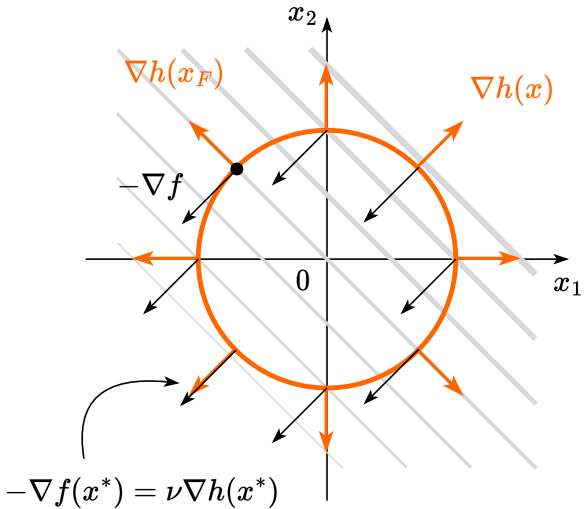
Then we came to the point of the budget set, moving from which it will not be possible to reduce our function. This is the local minimum in the constrained problem :)

Optimization with equality constraints



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$\langle y, \nabla^2_{xx} L(x^*, \nu^*) y \rangle > 0,$

$\forall y \neq 0 \in \mathbb{R}^n : \nabla h(x^*)^\top y = 0$

We should notice that $L(x^*, \nu^*) = f(x^*)$.

Equality constrained problem

$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } h_i(x) = 0,\ i = 1, \ldots, p \tag{ECP}$$

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

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

$$\nabla_x L(x^*, \nu^*) = 0$$
$$\nabla_\nu L(x^*, \nu^*) = 0$$

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):

- $m < n$

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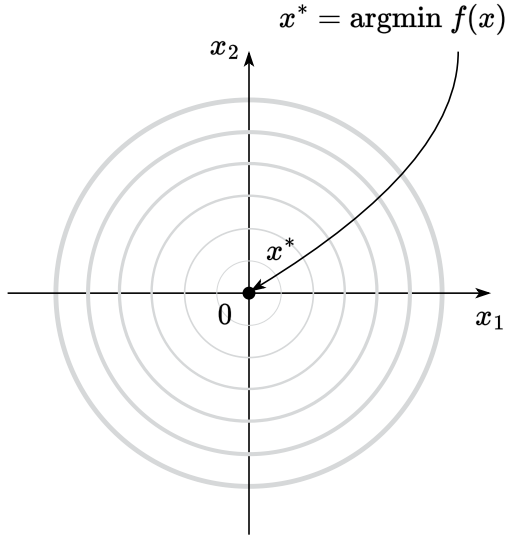
Optimization with inequality constraints

Example of inequality constraints

$$f(x) = x_1^2 + x_2^2 \quad g(x) = x_1^2 + x_2^2 - 1$$

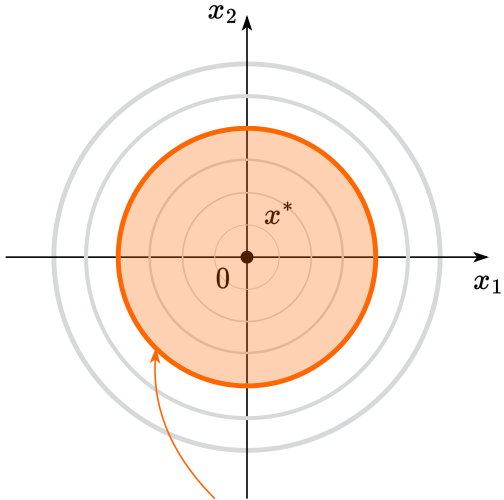
$$\begin{aligned} f(x) &\to \min_{x \in \mathbb{R}^n} \\ \text{s.t. } g(x) &\leq 0 \end{aligned}$$

Optimization with inequality constraints



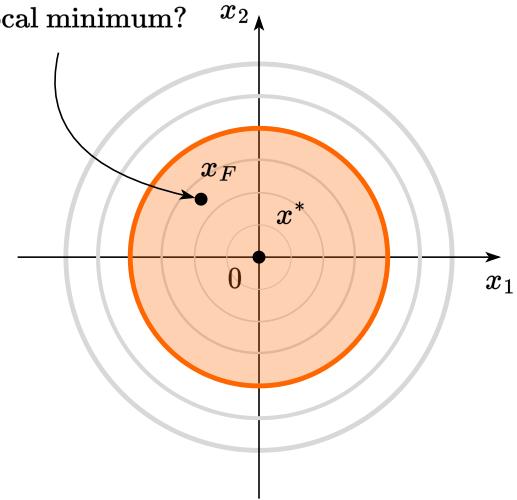
Contour lines of $f(x) = x_1^2 + x_2^2 = C$

Optimization with inequality constraints



Optimization with inequality constraints

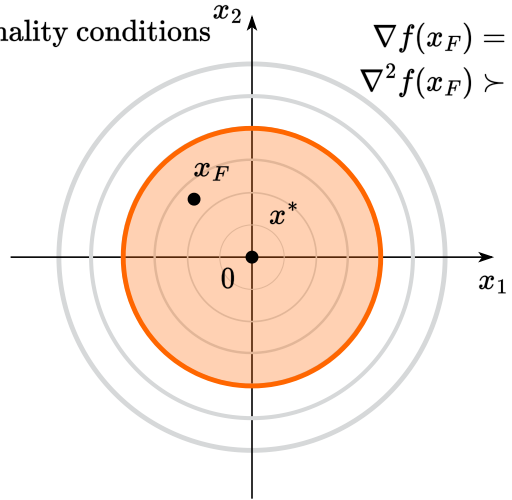
How to recognize that some feasible point is at local minimum?



Optimization with inequality constraints

Easy in this case! Just check unconstrained optimality conditions

$$\nabla f(x_F) = 0$$
$$\nabla^2 f(x_F) \succ 0$$



Optimization with inequality constraints

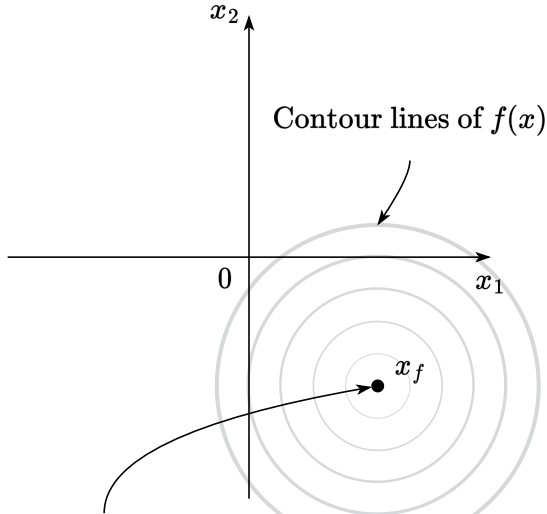
Thus, if the constraints of the type of inequalities are inactive in the constrained problem, then don't worry and write out the solution to the unconstrained problem. However, this is not the whole story. Consider the second childish example

$$f(x) = (x_1 - 1)^2 + (x_2 + 1)^2 \quad g(x) = x_1^2 + x_2^2 - 1$$

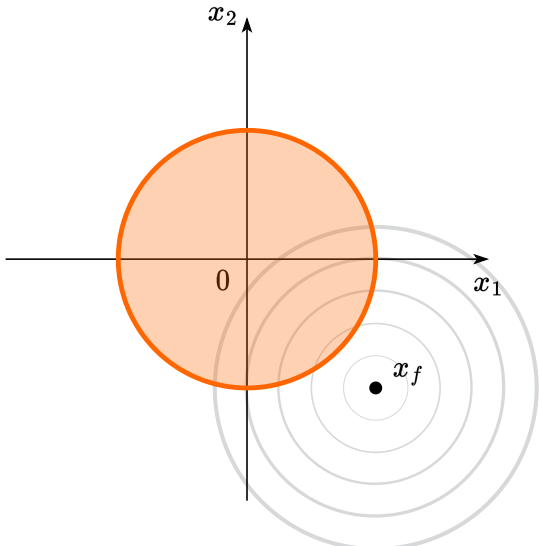
$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } g(x) \leq 0$$

Optimization with inequality constraints

$$f(x) = (x_1 - 1)^2 + (x_2 + 1)^2 = C$$



Optimization with inequality constraints



Optimization with inequality constraints

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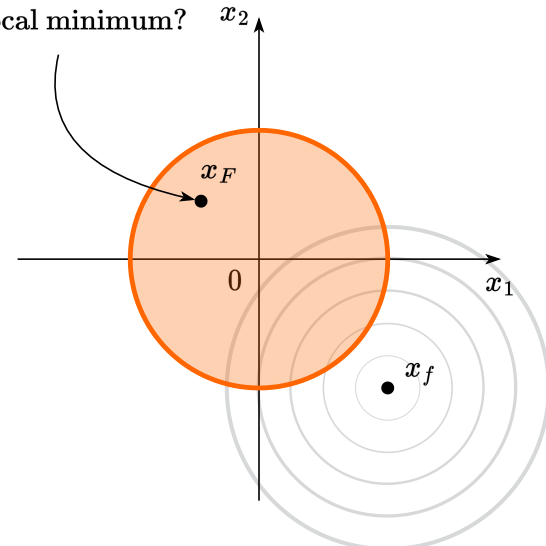
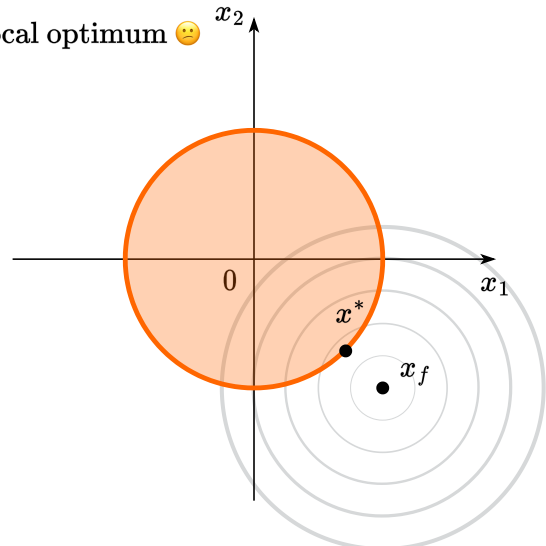


Optimization with inequality constraints

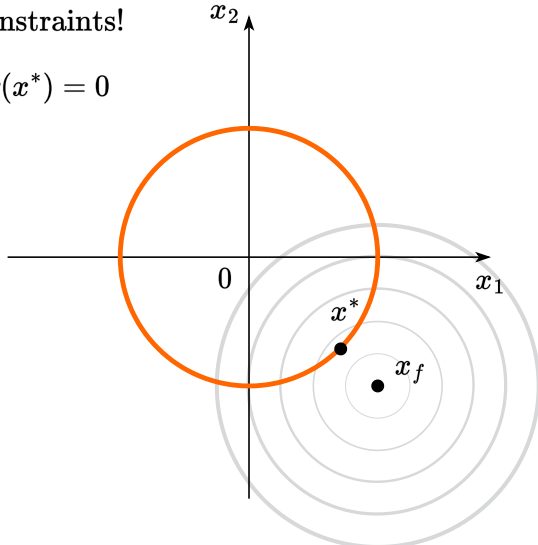
Not very easy in this case! Even gradient $\neq 0$ at local optimum 😐



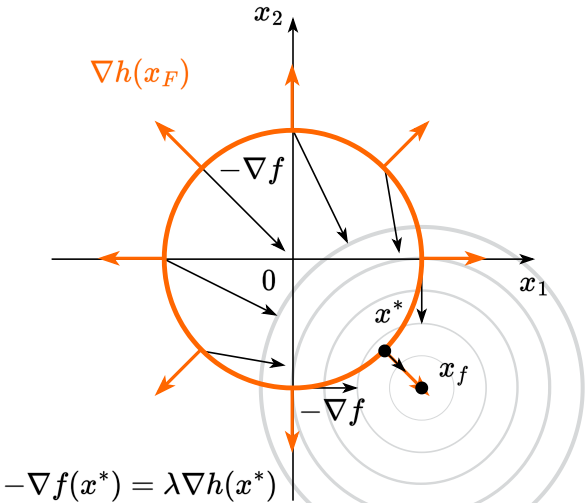
Optimization with inequality constraints

Effectively have a problem with equality constraints!

$g(x^*) = 0$



Optimization with inequality constraints



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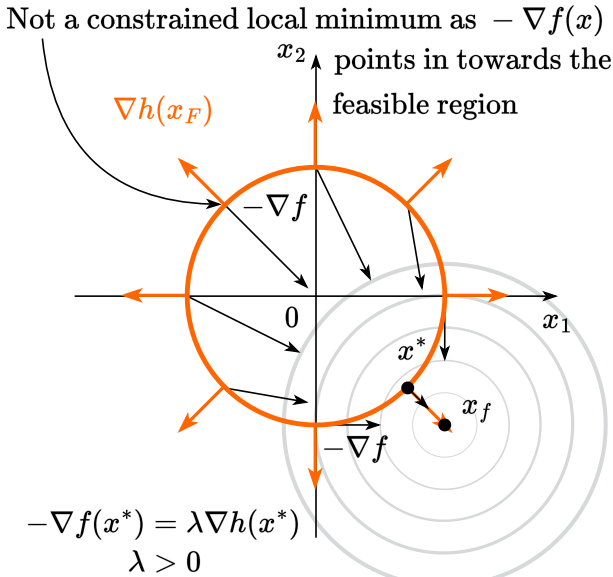

Optimization with inequality constraints

So, we have a problem:

$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } g(x) \leq 0$$

Two possible cases:

$g(x) \leq 0$ is inactive. $g(x^*) < 0$

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So, we have a problem:

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Lagrange function for inequality constraints

Combining two possible cases, we can write down the general conditions for the problem:

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Let's define the Lagrange function:

$$L(x, \lambda) = f(x) + \lambda g(x)$$

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General formulation

$$
\begin{aligned}
& f_0(x) \to \min_{x \in \mathbb{R}^n} \\
\text{s.t. } & f_i(x) \leq 0,\ i = 1, \ldots, m \\
& h_i(x) = 0,\ i = 1, \ldots, p
\end{aligned}
$$

This formulation is a general problem of mathematical programming.

The solution involves constructing a Lagrange function:

$$
L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)
$$

Necessary conditions

Let x^*, (λ^*, ν^*) be a solution to a mathematical programming problem with zero duality gap (the optimal value for the primal problem p^* is equal to the optimal value for the dual problem d^*). Let also the functions f_0, f_i, h_i be differentiable.

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Some regularity conditions

These conditions are needed to make KKT solutions the necessary conditions. Some of them even turn necessary conditions into sufficient (for example, Slater's). Moreover, if you have regularity, you can write down necessary second order conditions $\langle y, \nabla^2_{xx} L(x^*, \lambda^*, \nu^*) y \rangle \geq 0$ with *semi-definite* hessian of Lagrangian.

- **Slater's condition.** If for a convex problem (i.e., assuming minimization, f_0, f_i are convex and h_i are affine), there exists a point x such that $h(x) = 0$ and $f_i(x) < 0$ (existence of a strictly feasible point), then we have a zero duality gap and KKT conditions become necessary and sufficient.

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- For other examples, see wiki.

Proof in simple case

Subdifferential form of KKT

Let X be a linear normed space, and let $f_j : X \to \mathbb{R}$, $j = 0, 1, \ldots, m$, be convex proper (it never takes on the value $-\infty$ and also is not identically equal to ∞) functions. Consider the problem

$$f_0(x) \to \min_{x \in X}$$
$$\text{s.t. } f_j(x) \leq 0,\ j = 1, \ldots, m$$

Let $x^* \in X$ be a minimum in problem above and the functions f_j, $j = 0, 1, \ldots, m$, be continuous at the point x^*. Then there exist numbers $\lambda_j \geq 0$, $j = 0, 1, \ldots, m$, such that

$$\sum_{j=0}^{m} \lambda_j = 1,$$

$$\lambda_j f_j(x^*) = 0, \quad j = 1, \ldots, m,$$

$$0 \in \sum_{j=0}^{m} \lambda_j \partial f_j(x^*).$$

Proof in simple case

Proof

1. Consider the function

$$f(x) = \max\{f_0(x) - f_0(x^*), f_1(x), \ldots, f_m(x)\}.$$

The point x^* is a global minimum of this function.
Indeed, if at some point $x_e \in X$ the inequality
$f(x_e) < 0$ were satisfied, it would imply that
$f_0(x_e) < f_0(x^*)$ and $f_j(x_e) < 0$, $j = 1, \ldots, m$,
contradicting the minimality of x^* in problem above.

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$$\partial f(x^*) = \text{conv} \left(\bigcup_{j \in I} \partial f_j(x^*) \right),$$

where $I = \{0\} \cup \{j : f_j(x^*) = 0, 1 \le j \le m\}$.

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4. Therefore, there exist $g_j \in \partial f_j(x^*)$, $j \in I$, such that

$$\sum_{j \in I} \lambda_j g_j = 0, \quad \sum_{j \in I} \lambda_j = 1, \quad \lambda_j \geq 0, \quad j \in I.$$

It remains to set $\lambda_j = 0$ for $j \notin I$.

Example. Projection onto a hyperplane

$$\min \frac{1}{2}\|\mathbf{x}-\mathbf{y}\|^2, \quad \text{s.t.} \quad \mathbf{a}^T\mathbf{x} = b.$$

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> **Question**
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- Numerical Optimization by Jorge Nocedal and Stephen J. Wright.