Subgradient. Optimality conditions

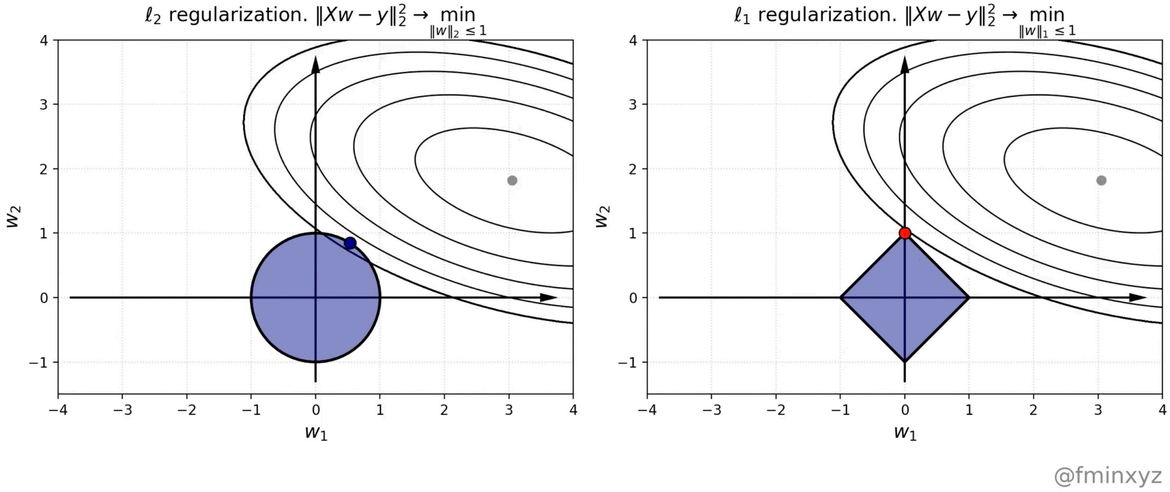
Daniil Merkulov

Optimization methods. MIPT

Subgradient and Subdifferential

ℓ_1-regularized linear least squares

ℓ_1 induces sparsity



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.

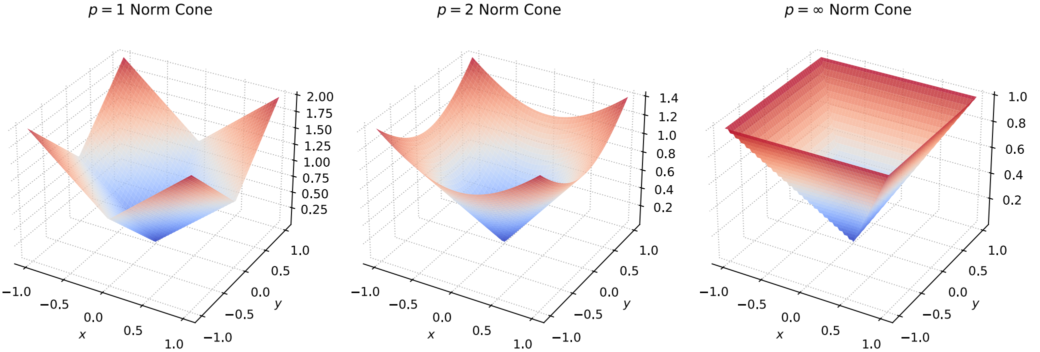


Figure 1: Norm cones for different p - norms are non-smooth

Convex function linear lower bound

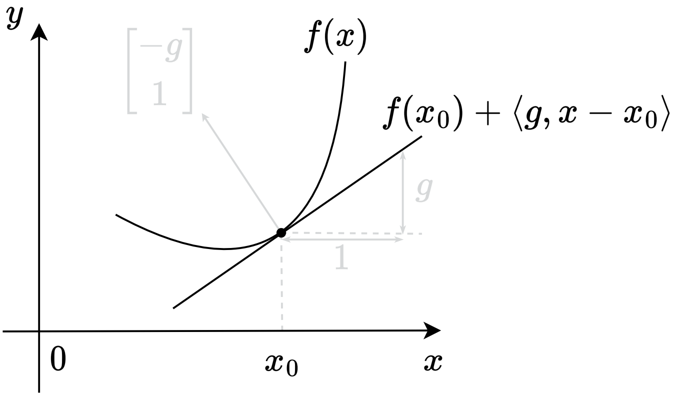


Figure 2: Taylor linear approximation serves as a global lower bound for a convex function

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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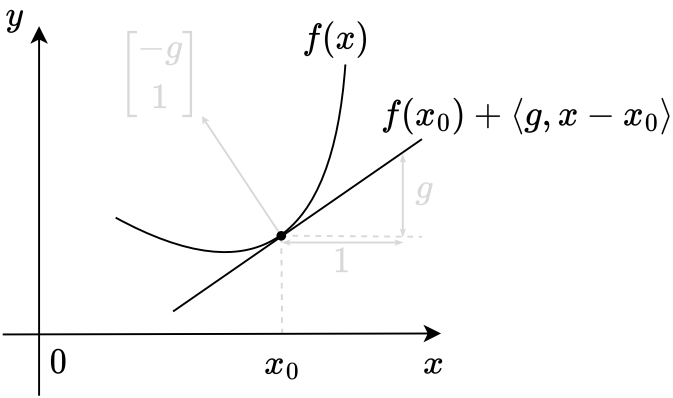

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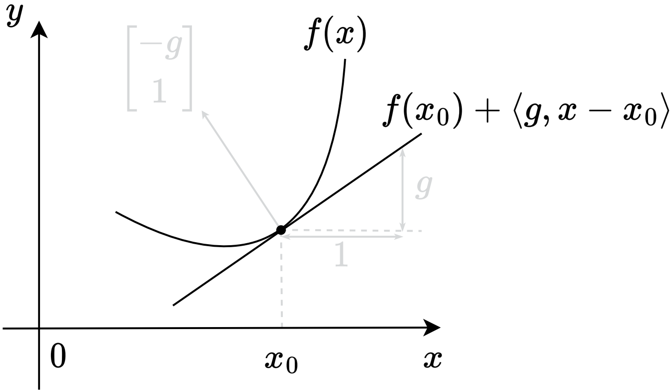
for some vector g, i.e., the tangent to the graph of the function is the *global* estimate from below for the function.

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

Convex function linear lower bound



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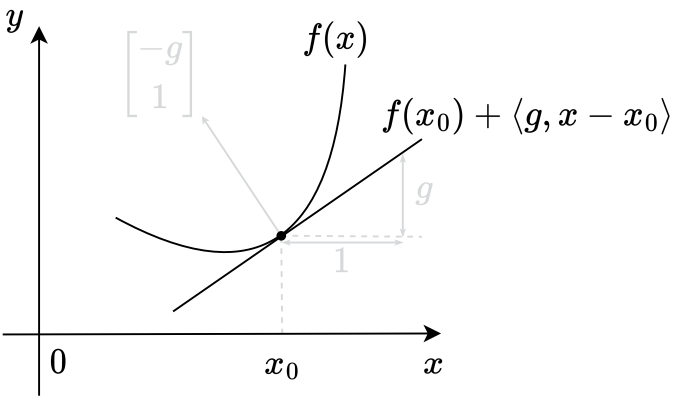

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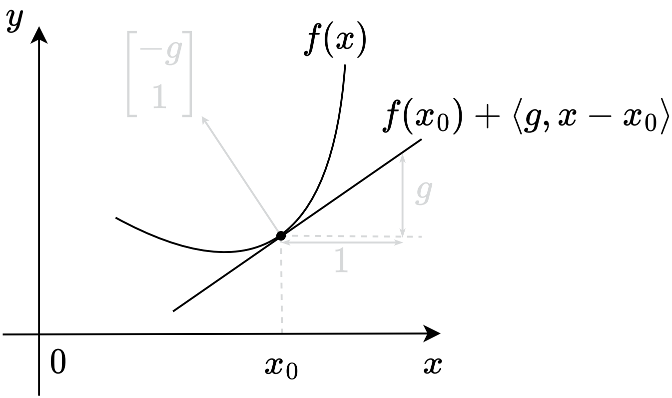

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We wouldn't want to lose such a nice property.

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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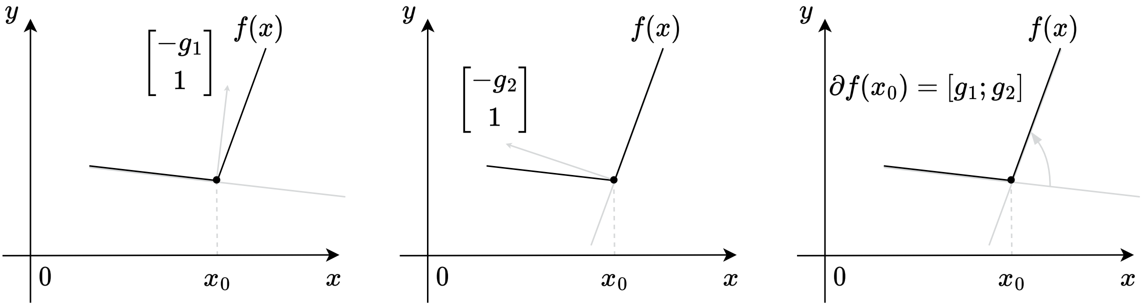

Figure 3: Subdifferential is a set of all possible subgradients

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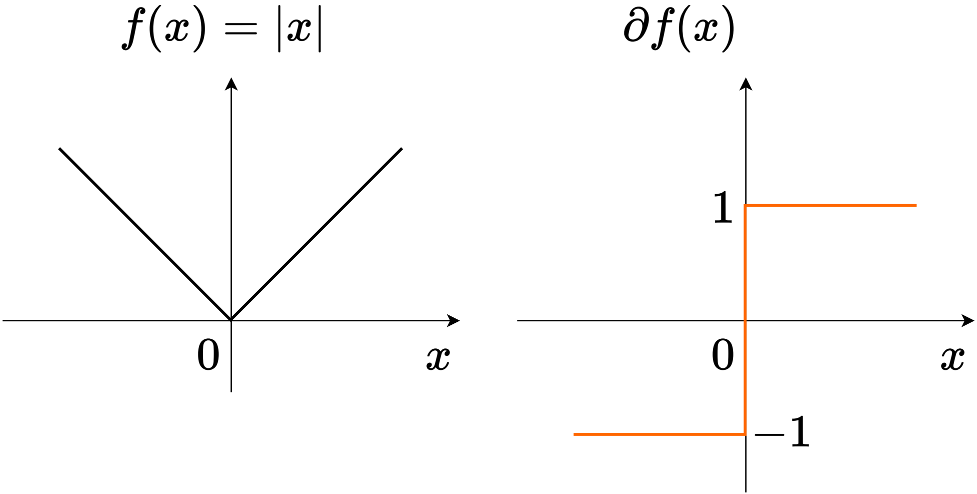

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Жадан Т. 1

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Beck First-ORDER Numerical methods

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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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which implies:

$$\frac{f(x_0 + tv) - f(x_0)}{t} \geq \langle s, v \rangle$$

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

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

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

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

leading to $s = \nabla f(x_0)$.

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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 $\nabla f(x_0) \in \partial f(x_0)$.

Subdifferentiability and convexity

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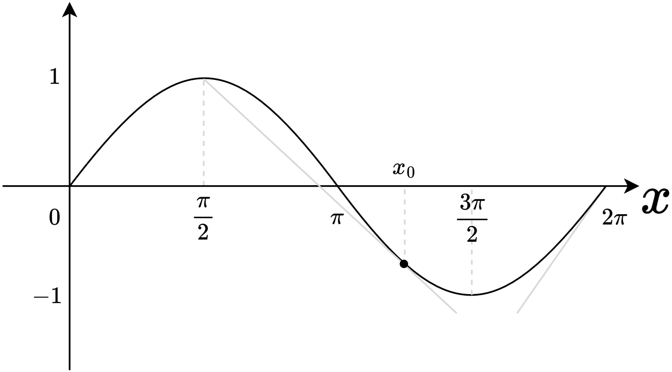
Find $\partial f(x)$, if $f(x) = \sin x, x \in [\pi/2; 2\pi]$



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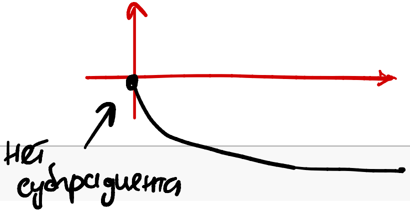

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Convexity follows from subdifferentiability at any point. A natural question to ask is whether the converse is true: is every convex function subdifferentiable? It turns out that, generally speaking, the answer to this question is negative.

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

$f: \mathbb{R}^n \to \mathbb{R}$

rint
relint
относит. внутр. (S):
$\{x \in S \mid \exists B_\varepsilon(x) \subseteq \text{aff}(S)\}$

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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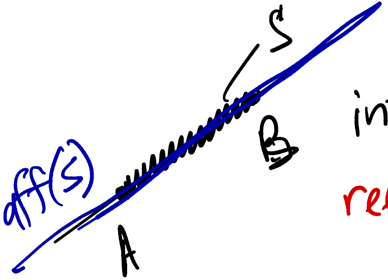

$\text{int}(S) = \emptyset$

relint(S)
отрезок без концов

$E \subseteq \mathbb{R}^n \quad f: E \to \mathbb{R}$

Subdifferential calculus

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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 $I_S : \mathbb{R}^n \to \mathbb{R}$,

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

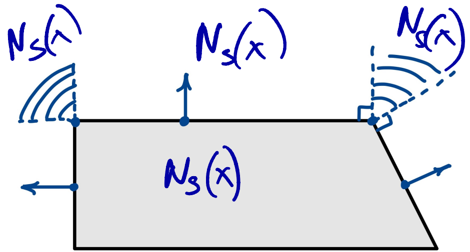
For $x \in S$, $\partial I_S(x) = \mathcal{N}_S(x)$, the **normal cone** of S at x is, recall

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

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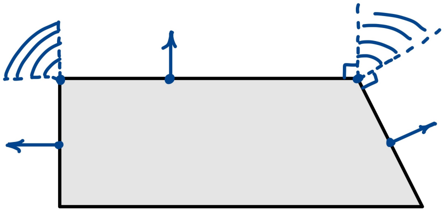
- For $y \in S$, this means $0 \geq g^T(y - x)$



Optimality Condition

Принцип Ферма

For any f (convex or not),

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

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

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

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

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

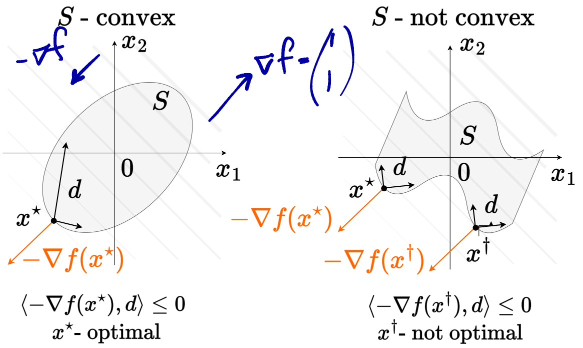
Intuitively: this says that the gradient increases as we move away from x. How to prove it? First, recast the problem as переход от условной задачи к безусловной

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

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 пусть f - выпуклая $\partial I_S(x) = N_S(x)$

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

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

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

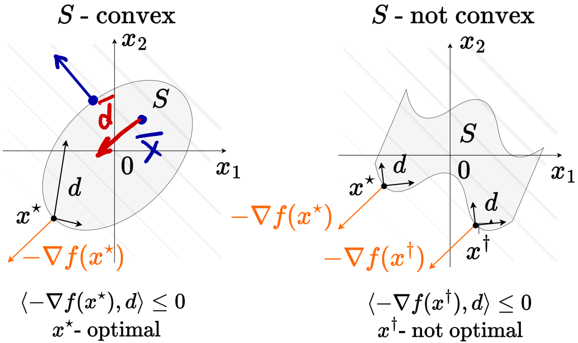
$$\Leftrightarrow -\nabla f(x)^T x \geq -\nabla f(x)^T y \text{ for all } y \in S$$

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

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).

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



Example 1

Example

Find $\partial f(x)$, if $f(x) = \underbrace{|x-1|}_{f_1} + \underbrace{|x+1|}_{f_2}$

$f: \mathbb{R} \to \mathbb{R}$

$= f_1(x) + f_2(x)$

$\partial f(x) = \partial f_1(x) + \partial f_2(x)$

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

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

Ответ:

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

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So

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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 $q \geq 1$.

$$f(x) = \varphi(\tilde{f_0}(x)) = \varphi(\max(0, f_0(x)))$$

где $\varphi(x) = x^q$, $x \geq 0$, $q \geq 1$

$$\tilde{f_0}(x) = \max(0, f_0(x))$$

$$\partial f = q \cdot [\max(0, f_0(x))]^{q-1} \cdot \partial \tilde{f_0}(x)$$

$$\partial \tilde{f_0}(x) = \text{conv}\left\{ \bigcup_{i:\, \tilde{f_0}(x) = g_i(x)} \{\underbrace{0}_{g_1}, \underbrace{\partial f(x)}_{g_2}\} \right\}$$

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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:

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

$$\max(0, f_0(x)) = \text{conv} \cup \left(\{0\}; \{\partial f_0(x)\}\right)$$

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

$$\langle s, x\rangle - \|x\| \leq \langle s, x_0\rangle - \|x_0\|, \text{ for all } x \in V,$$

or equivalently,

$$\sup_{x \in V}\{\langle s, x\rangle - \|x\|\} \leq \langle s, x_0\rangle - \|x_0\|.$$

By the definition of the supremum, the latter is equivalent to

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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

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

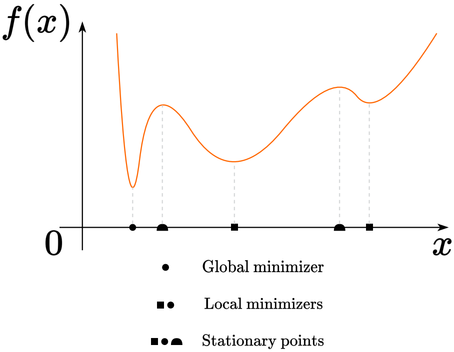
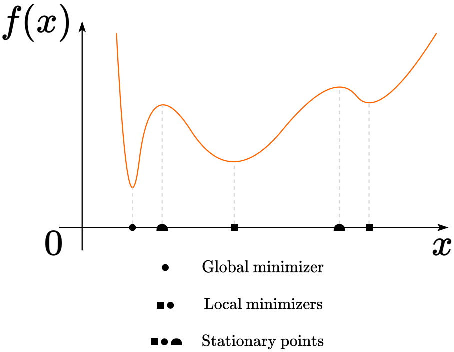


Figure 5: Illustration of different stationary (critical) points

Background



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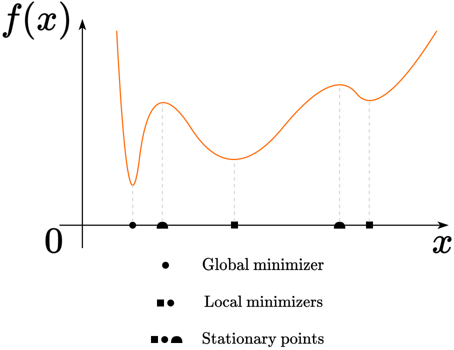

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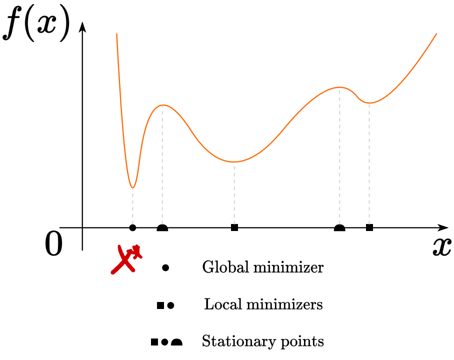

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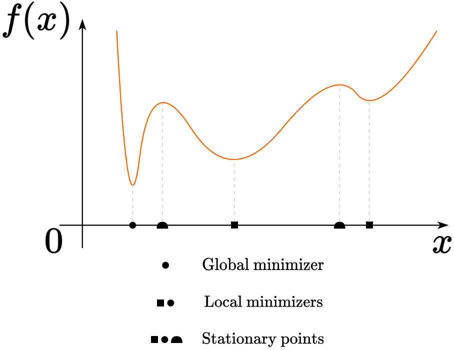

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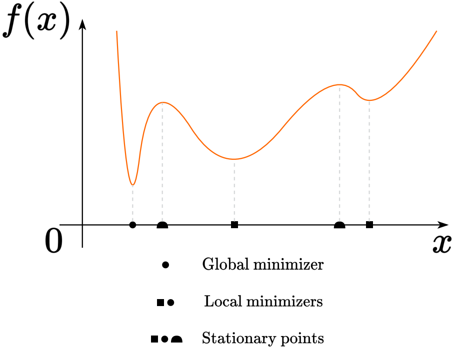

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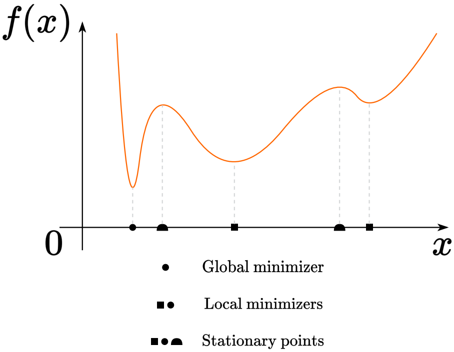

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- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

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

Extreme value (Weierstrass) theorem

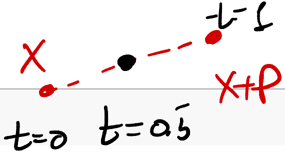

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Figure 6: A lot of practical problems are theoretically solvable

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:

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

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

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

БЕЗУСЛОВНАЯ

$0 \in \partial f(x^*)$

Unconstrained optimization

ОПТИМИЗАЦИЯ

$S = \mathbb{R}^n$

Necessary Conditions

Необх. усл. лок. экстремума

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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$$p^T \nabla f(x^*) = -\|\nabla f(x^*)\|^2 < 0$$

Пусть x^* - минимум, но $\nabla f(x^*) \neq 0$

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For any $\bar{t} \in (0, T]$, we have by Taylor's theorem that

Формула Тейлора!

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

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

Therefore, $\boxed{f(x^* + \bar{t}p) < f(x^*)}$ 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.

ч.т.д.

Sufficient Conditions

Second-Order Sufficient Conditions

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

СТРОГО

$$\nabla f(x^*) = 0 \quad \nabla^2 f(x^*) \succ 0.$$

Then x^* is a strict local minimizer of f.

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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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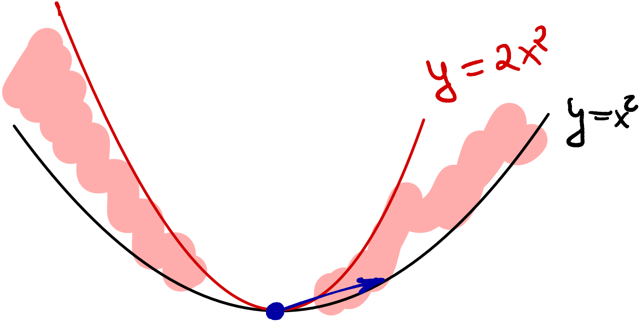
Although the surface does not have a local minimizer at the origin, its intersection with any vertical plane through the origin (a plane with equation $y = mx$ or $x = 0$) is a curve that has a local minimum at the origin. In other words, if a point starts at the origin $(0,0)$ of the plane, and moves 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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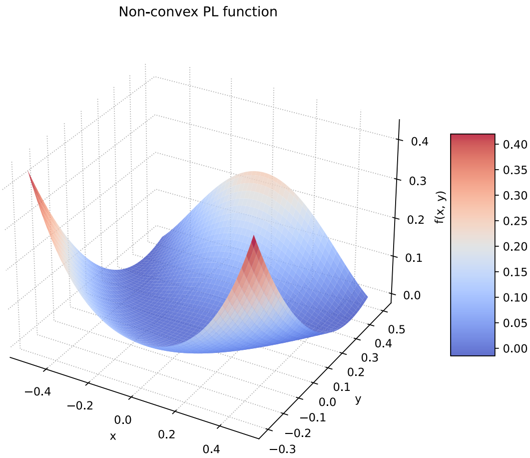

Условная оптимизация

Constrained optimization

$$S \neq \mathbb{R}^n$$

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

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.

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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$$-\nabla f(x^*) \in N_S(x^*)$$

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

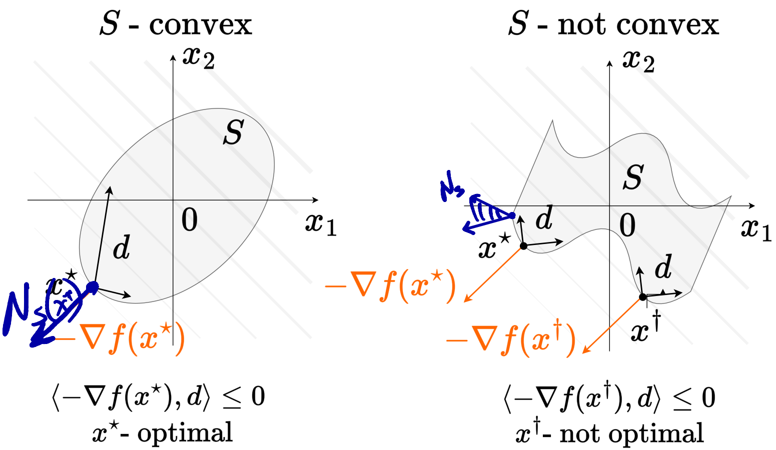

Figure 7: General first order local optimality condition

Convex case

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

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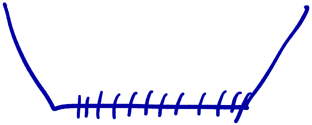
- Any local minima is the global one.



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

Optimization with equality constraints

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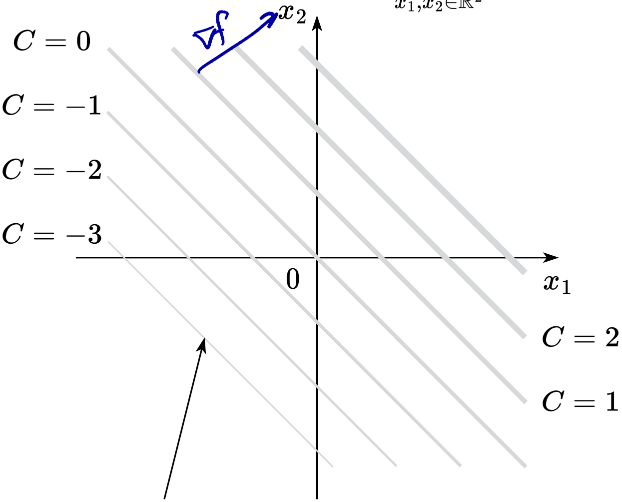
We will try to illustrate an approach to solve this problem through the simple example with $f(x) = x_1 + x_2$ and $h(x) = x_1^2 + x_2^2 - 2$.

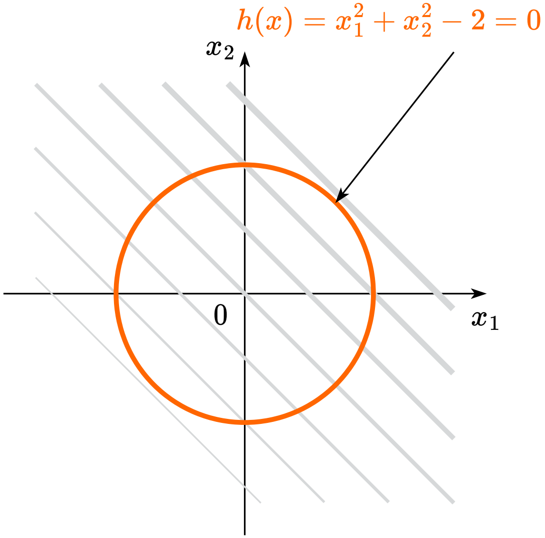
Optimization with equality constraints

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



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

Optimization with equality constraints



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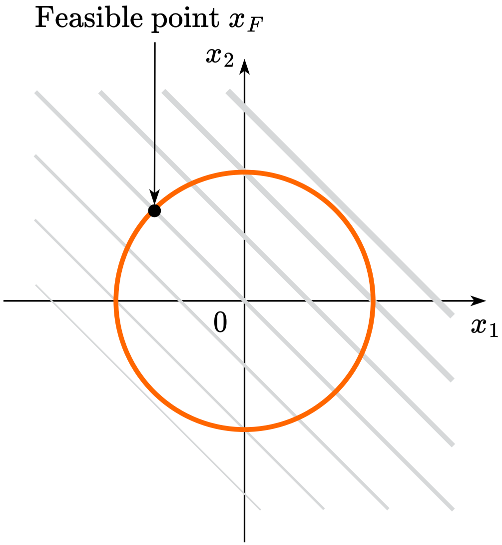

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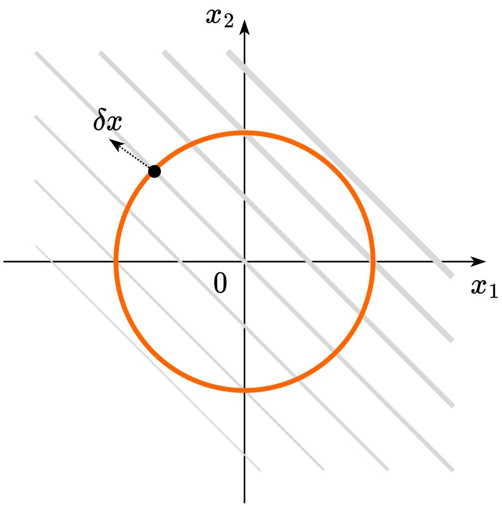

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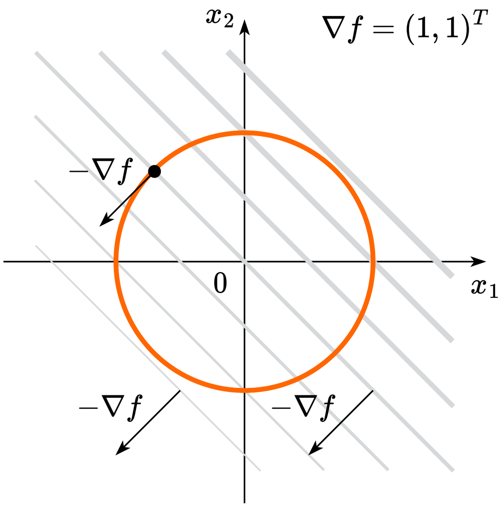

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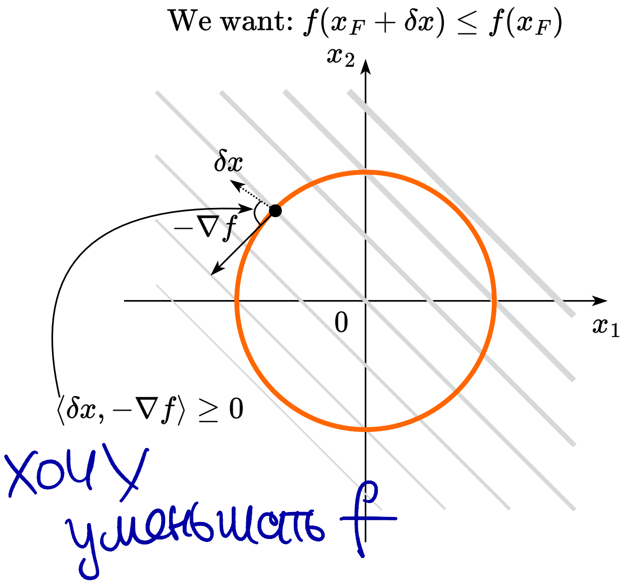
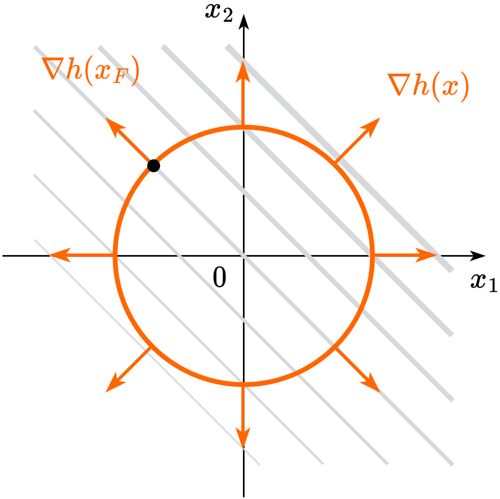
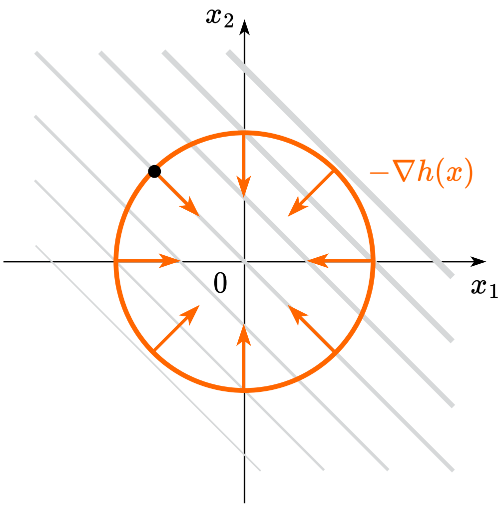


Optimization with equality constraints

$$\nabla h = (2x_1, 2x_2)^T$$

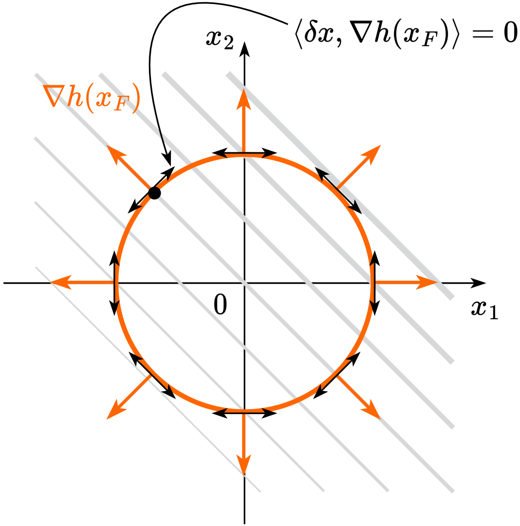


Optimization with equality constraints



Optimization with equality constraints

Хочу остаться в S



Optimization with equality constraints

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требования к δx

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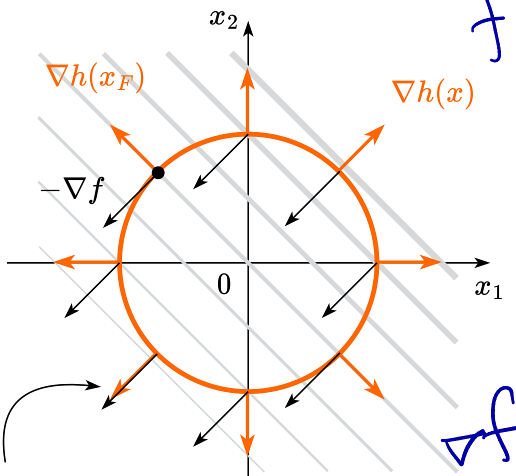
Then we came to the point of the budget set, moving from which it will not be possible to reduce our function. This is the local minimum in the constrained problem :)

Optimization with equality constraints



$$-\nabla f(x^*) = \nu \nabla h(x^*)$$

$f(x^*) + \nu \cdot h(x^*)$

$\nabla f(x^*) + \nu \nabla h(x^*) = 0$

Lagrangian

So let's define a Lagrange function (just for our convenience):

$$L(x, \nu) = f(x) + \nu h(x)$$

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$\nabla_x L = \nabla f(x^*) + \nu \nabla h(x^*) = 0$

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$L: \mathbb{R}^{n+1} \to \mathbb{R}$

$$L(x, \nu) = f(x) + \nu h(x)$$

$L(x, \nu)$

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

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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

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

ν – множители Лагранжа

Функция Лагранжа →

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

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

$$
\begin{cases}
\nabla_x L(x^*, \nu^*) = 0 \\
\nabla_\nu L(x^*, \nu^*) = 0
\end{cases}
$$

ECP: Sufficient conditions

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

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

Linear Least Squares

$\frac{1}{2}\|x\|_2^2 \to \min\limits_{x \in \mathbb{R}^n}$

$Ax = b$

$Ax = b \quad m < n$ Недоопр. система

$A^\dagger = A^T(AA^T)^{-1}$ \dagger

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):

- $m < n$

$x^* = A^T(AA^T)^{-1}b$

$\sum \nu_i \cdot (Ax - b)_i = \nu^T x$

Решение: 1) $L(x) = f(x) + \nu h(x) = \frac{1}{2}\|x\|_2^2 + \nu^T(Ax - b)$

2) $\nabla_x L = 2 \cdot \frac{1}{2} \cdot x + A^T\nu = 0$

$\nabla_\nu L = Ax - b = 0$

$\begin{cases} x = -A^T\nu \\ Ax = b \end{cases} \quad \begin{cases} x = -A^T\nu \\ A \cdot (-A^T\nu) = b \end{cases} \quad \begin{cases} x = +A^T(AA^T)^{-1}b \\ \nu = -(AA^T)^{-1}b \end{cases}$

m×n n×m m×m

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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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):

- $m < n$
- $m = n$
- $m > n$

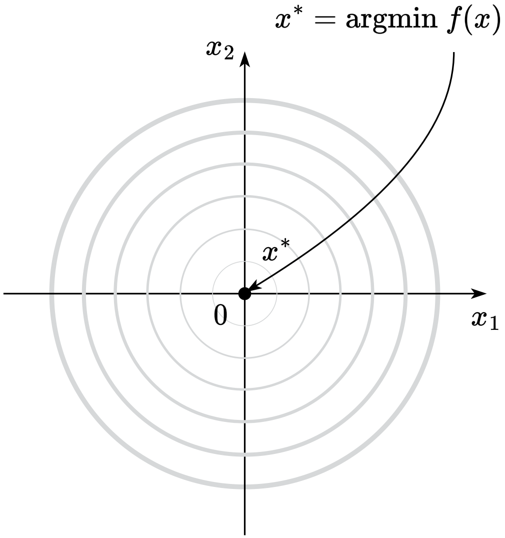
Optimization with inequality constraints

Example of inequality constraints

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

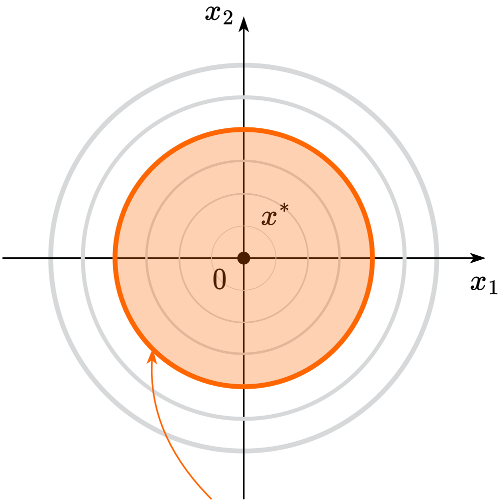
$$f(x) \to \min_{x \in \mathbb{R}^n}$$
$$\text{s.t. } g(x) \leq 0$$

Optimization with inequality constraints



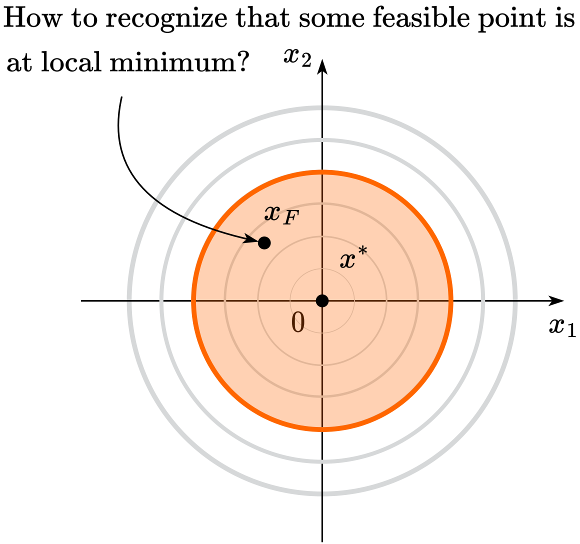
Contour lines of $f(x) = x_1^2 + x_2^2 = C$

Optimization with inequality constraints



Feasible region $g(x) = x_1^2 + x_2^2 - 1 \leq 0$

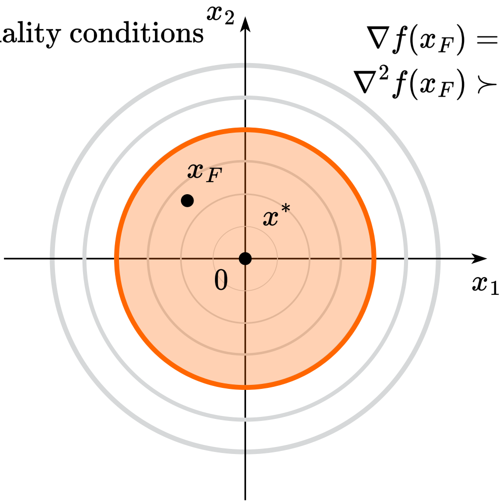
Optimization with inequality constraints



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

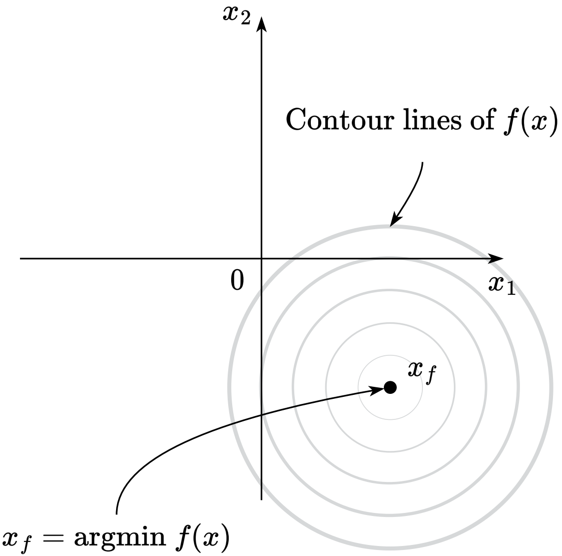
Thus, if the constraints of the type of inequalities are inactive in the constrained problem, then don't worry and write out the solution to the unconstrained problem. However, this is not the whole story. Consider the second childish example

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

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

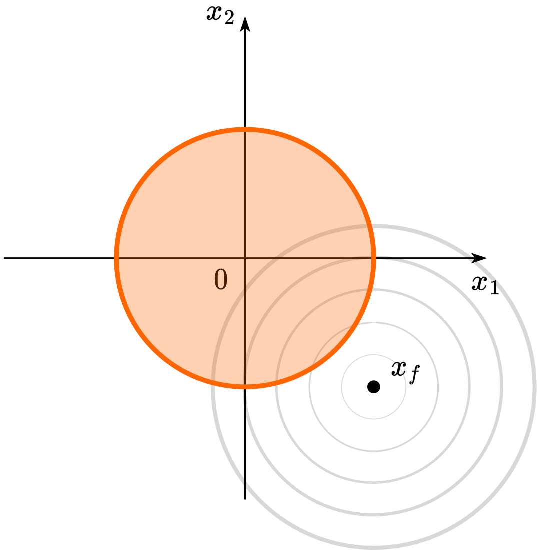
Optimization with inequality constraints

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



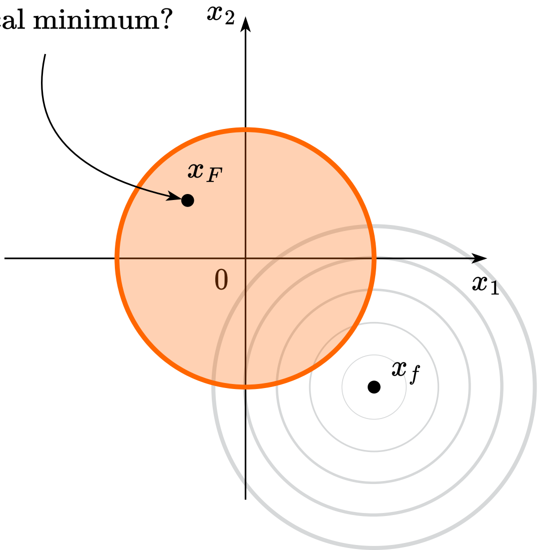
Optimization with inequality constraints

Feasible region $g(x) = x_1^2 + x_2^2 - 1 \leq 0$



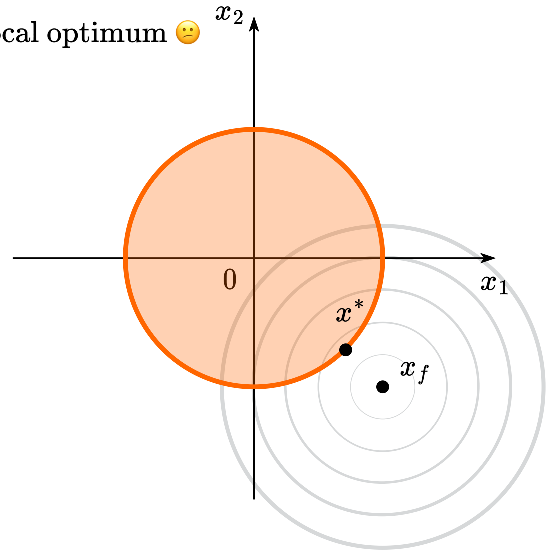
Optimization with inequality constraints

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



Optimization with inequality constraints

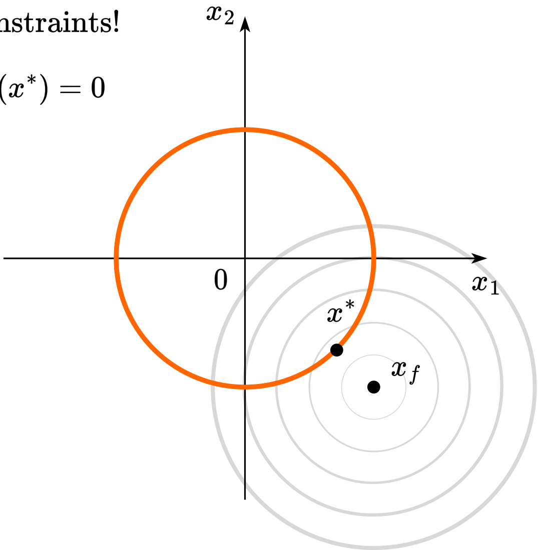
Not very easy in this case! Even gradient $\neq 0$ at local optimum 😕



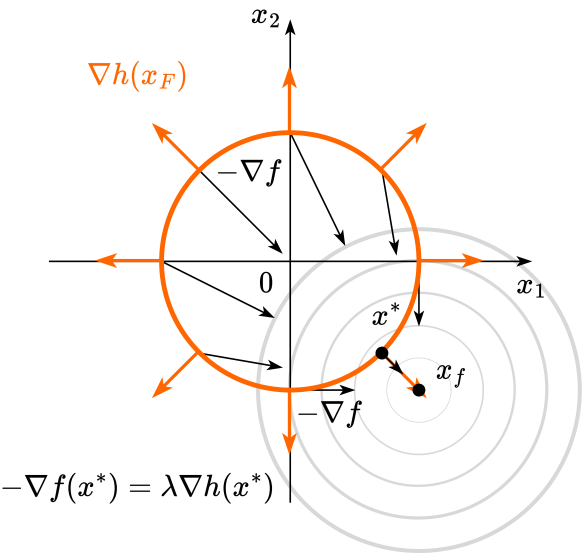
Optimization with inequality constraints

Effectively have a problem with equality constraints!

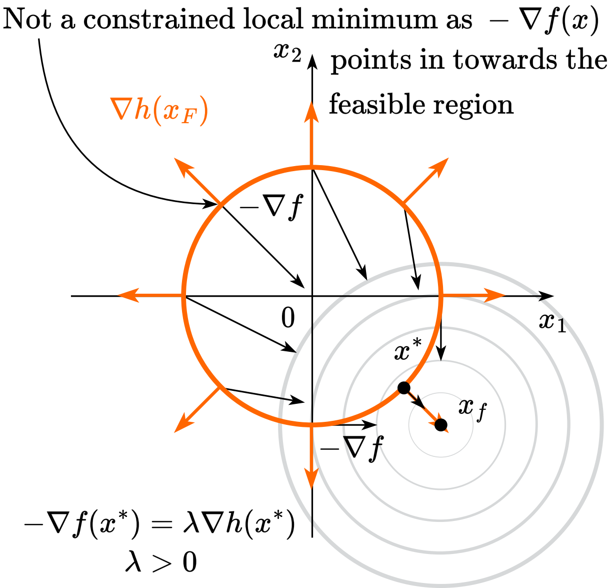
$$g(x^*) = 0$$



Optimization with inequality constraints



Optimization with inequality constraints



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. $g(x^*) < 0$

- $g(x^*) < 0$

Optimization with inequality constraints

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- $g(x^*) < 0$
- $\nabla f(x^*) = 0$

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$$
\text{s.t. } g(x) \leq 0
$$

Two possible cases:

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

- $g(x^*) < 0$
- $\nabla f(x^*) = 0$
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Optimization with inequality constraints

So, we have a problem:

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

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- $g(x^*) = 0$
- Necessary conditions: $-\nabla f(x^*) = \lambda \nabla g(x^*)$, $\lambda > 0$
- Sufficient conditions:
  $\langle y, \nabla^2_{xx} L(x^*, \lambda^*) y \rangle > 0, \forall y \neq 0 \in \mathbb{R}^n : \nabla g(x^*)^\top y = 0$

Lagrange function for inequality constraints

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

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

Let's define the Lagrange function:

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

The classical Karush-Kuhn-Tucker first and second-order optimality conditions for a local minimizer x^*, stated under some regularity conditions, can be written as follows.

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If x^* is a local minimum of the problem described above, then there exists a unique Lagrange multiplier λ^* such that:

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(1)\ \nabla_x L(x^*, \lambda^*) = 0
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$I(x^*) = \{ i \mid g_i(x^*) = 0 \}$

General formulation

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

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

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

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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3. By the Dubovitskii-Milyutin theorem, we have

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

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

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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

$$
\min \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \text{s.t.} \quad \mathbf{a}^T\mathbf{x} = b.
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$$\min \frac{1}{2}\|x - y\|^2, \quad \text{s.t.} \quad x^\top 1 = 1, \quad x \geq 0. \quad x$$

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- $\frac{\partial L}{\partial x_i} = x_i - y_i - \lambda_i + \nu = 0$

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> **Question**
>
> Solve the above conditions in $O(n \log n)$ time.

Example. Projection onto simplex

$$\min_x \frac{1}{2}\|x - y\|^2, \quad \text{s.t.} \quad x^\top 1 = 1, \quad x \geq 0.$$

KKT Conditions

The Lagrangian is given by:

$$L = \frac{1}{2}\|x - y\|^2 - \sum_i \lambda_i x_i + \nu(x^\top 1 - 1)$$

Taking the derivative of L with respect to x_i and writing KKT yields:

- $\frac{\partial L}{\partial x_i} = x_i - y_i - \lambda_i + \nu = 0$
- $\lambda_i x_i = 0$
- $\lambda_i \geq 0$
- $x^\top 1 = 1, \quad x \geq 0$

> **Question**
>
> Solve the above conditions in $O(n \log n)$ time.

> **Question**
>
> Solve the above conditions in $O(n)$ time.

References

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- Numerical Optimization by Jorge Nocedal and Stephen J. Wright.