Recap of Conjugate sets, conjugate functions. Subgradient and subdifferential

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Optimization methods. MIPT

Conjugate sets

Conjugate set

Let $S \subseteq \mathbb{R}^n$ be an arbitrary non-empty set. Then its conjugate set is defined as:

$$S^* = \{y \in \mathbb{R}^n \mid \langle y, x\rangle \geq -1 \;\; \forall x \in S\}$$

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- The sets S_1 and S_2 are called **inter-conjugate** if $S_1^* = S_2, S_2^* = S_1$.

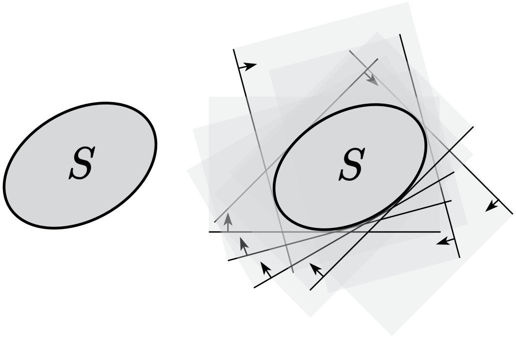

Figure 1: Convex sets may be described in a dual way - through the elements of the set and through the set of hyperplanes supporting it

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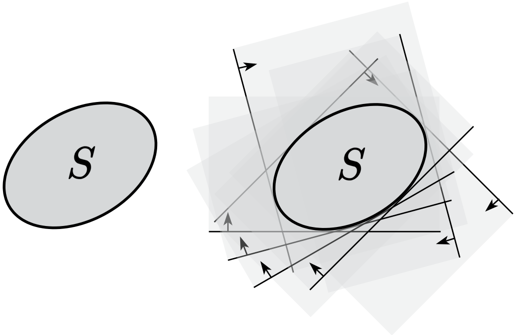
- A set S is called **self-conjugate** if $S^* = S$.



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- $S^* = \left(\overline{S}\right)^*$.

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- $S \subset \overline{S} \to \left(\overline{S}\right)^* \subset S^*$.
- Let $p \in S^*$ and $x_0 \in \overline{S}, x_0 = \lim\limits_{k \to \infty} x_k$. Then by virtue of the continuity of the function $f(x) = p^T x$, we have: $p^T x_k \geq -1 \to p^T x_0 \geq -1$. So $p \in \left(\overline{S}\right)^*$, hence $S^* \subset \left(\overline{S}\right)^*$.

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- Let $p \in S^*$, $x_0 \in \mathbf{conv}(S)$, i.e., $x_0 = \sum\limits_{i=1}^k \theta_i x_i \mid x_i \in S, \sum\limits_{i=1}^k \theta_i = 1, \theta_i \geq 0$.

  So $p^T x_0 = \sum\limits_{i=1}^k \theta_i p^T x_i \geq \sum\limits_{i=1}^k \theta_i (-1) = 1 \cdot (-1) = -1$. So $p \in (\mathbf{conv}(S))^*$, hence $S^* \subset (\mathbf{conv}(S))^*$.

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- From all points of the ball X, take such a point $x \in X$ that its scalar product of p: $p^T x$ is minimal, then this is the point $x = -\frac{p}{\|p\|} r$.

$$p^T x = p^T \left(-\frac{p}{\|p\|} r \right) = -\|p\| r \geq -1$$

$$\|p\| \leq \frac{1}{r} \in Y$$

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- Now let $p \in Y$. We need to show that $p \in X^*$, i.e., $\langle p, x \rangle \geq -1$. It's enough to apply the Cauchy-Bunyakovsky inequality:

$$\|\langle p, x \rangle\| \leq \|p\| \|x\| \leq \frac{1}{r} \cdot r = 1$$

The latter comes from the fact that $p \in B(0, 1/r)$ and $x \in B(0, r)$.
So $Y \subset X^*$.

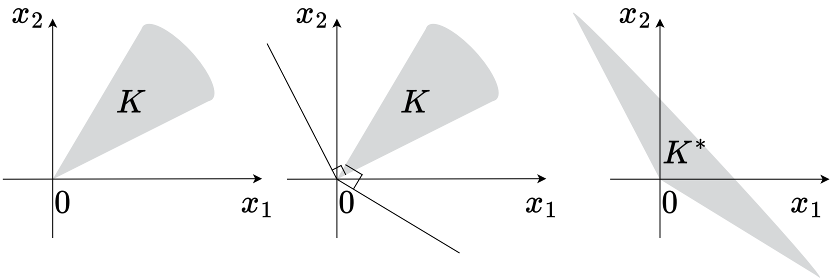
Dual cone

A conjugate cone to a cone K is a set K^* such that:

$$K^* = \{y \mid \langle x, y\rangle \geq 0 \quad \forall x \in K\}$$

To show that this definition follows directly from the definitions above, recall what a conjugate set is and what a cone $\forall \lambda > 0$ is.

$$\{y \in \mathbb{R}^n \mid \langle y, x\rangle \geq -1 \;\; \forall x \in S\} \to \{\lambda y \in \mathbb{R}^n \mid \langle y, x\rangle \geq -\frac{1}{\lambda} \;\; \forall x \in S\}$$



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- Let $K_1, \ldots, K_m$ be cones in $\mathbb{R}^n$. Let also their intersection have an interior point, then:

$$\left(\bigcap_{i=1}^m K_i \right)^* = \sum_{i=1}^m K_i^*$$

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Find the conjugate cone for a monotone nonnegative cone:

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Note that:

$$\sum_{i=1}^{n} x_i y_i = y_1(x_1 - x_2) + (y_1 + y_2)(x_2 - x_3) + \ldots + (y_1 + y_2 + \ldots + y_{n-1})(x_{n-1} - x_n) + (y_1 + \ldots + y_n)x_n$$

Since in the presented sum in each summand, the second multiplier in each summand is non-negative, then:

$$y_1 \geq 0, \quad y_1 + y_2 \geq 0, \quad \ldots, \quad y_1 + \ldots + y_n \geq 0$$

So $K^* = \left\{ y \mid \sum_{i=1}^{k} y_i \geq 0, k = \overline{1, n} \right\}$.

Polyhedra

The set of solutions to a system of linear inequalities and equalities is a polyhedron:

$$Ax \preceq b, \quad Cx = d$$

Here $A \in \mathbb{R}^{m \times n}, C \in \mathbb{R}^{p \times n}$, and the inequality is a piecewise inequality.

Theorem

Let $x_1, \ldots, x_m \in \mathbb{R}^n$. Conjugate to a polyhedral set:

$$S = \mathbf{conv}(x_1, \ldots, x_k) + \mathbf{cone}(x_{k+1}, \ldots, x_m)$$

is a polyhedron (polyhedron):

$$S^* = \left\{ p \in \mathbb{R}^n \mid \langle p, x_i \rangle \geq -1, i = \overline{1,k}; \langle p, x_i \rangle \geq 0, i = \overline{k+1,m} \right\}$$

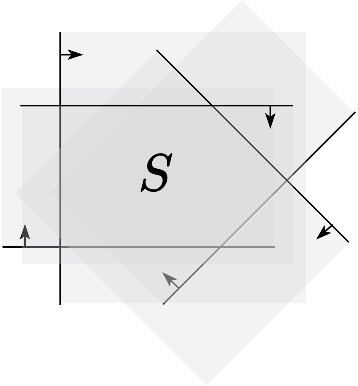

Figure 3: Polyhedra

Proof

- Let $S = X, S^* = Y$. Take some $p \in X^*$, then $\langle p, x_i \rangle \geq -1, i = \overline{1, k}$. At the same time, for any $\theta > 0, i = \overline{k+1, m}$:

$$
\langle p, x_i \rangle \geq -1 \to \langle p, \theta x_i \rangle \geq -1
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\langle p, x_i \rangle \geq -\frac{1}{\theta} \to \langle p, x_i \rangle \geq 0.
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So $p \in Y \to X^* \subset Y$.

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  So $p \in Y \to X^* \subset Y$.

- Suppose, on the other hand, that $p \in Y$. For any point $x \in X$:

$$
x = \sum_{i=1}^m \theta_i x_i \qquad \sum_{i=1}^k \theta_i = 1, \theta_i \geq 0
$$

  So:

$$
\langle p, x \rangle = \sum_{i=1}^m \theta_i \langle p, x_i \rangle = \sum_{i=1}^k \theta_i \langle p, x_i \rangle + \sum_{i=k+1}^m \theta_i \langle p, x_i \rangle \geq \sum_{i=1}^k \theta_i (-1) + \sum_{i=1}^k \theta_i \cdot 0 = -1.
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Conjugate functions

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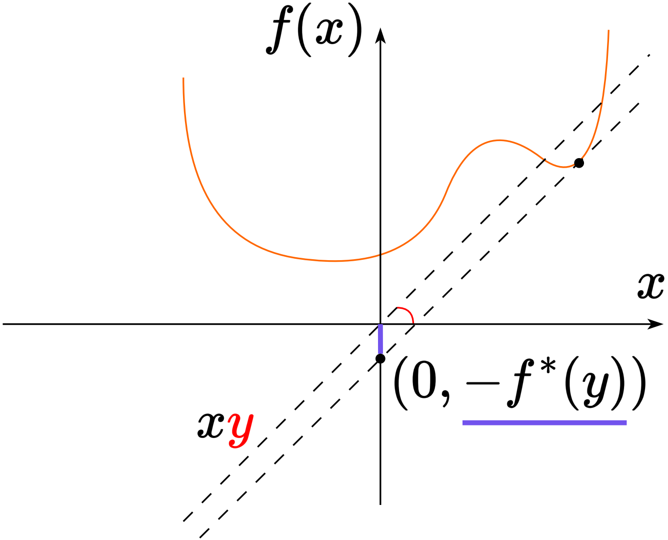

Recall that given $f : \mathbb{R}^n \to \mathbb{R}$, the function defined by

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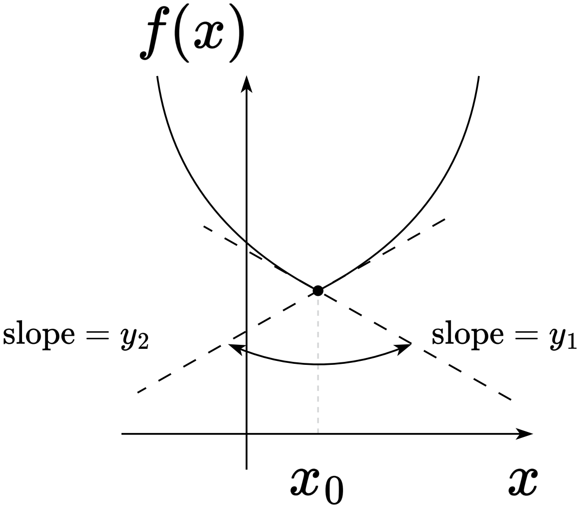

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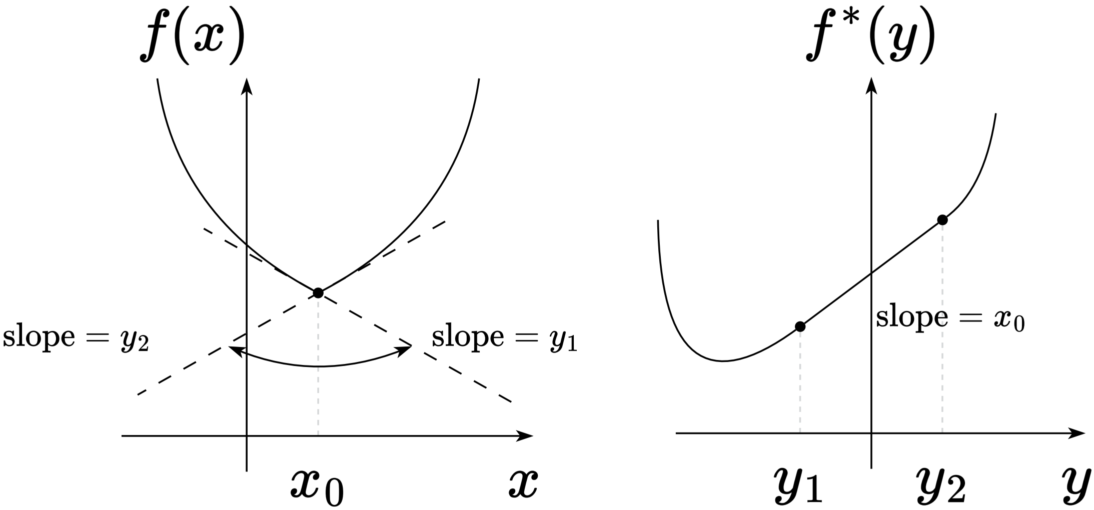
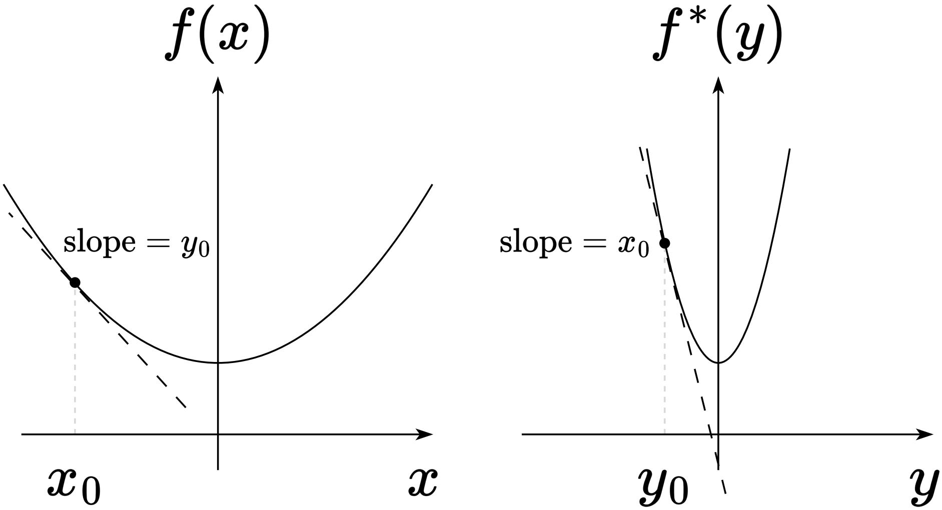


Slopes of f and f^*



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Hence, defining $x_u = \nabla f^*(u)$ and $x_v = \nabla f^*(v)$,

$$f(x_v) - u^T x_v \geq f(x_u) - u^T x_u + \frac{\mu}{2}\|x_u - x_v\|^2$$
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Adding these together, using the Cauchy-Schwarz inequality, and rearranging shows that

$$\|x_u - x_v\|^2 \leq \frac{1}{\mu}\|u - v\|^2$$

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Proof of "$\Leftarrow$": for simplicity, call $g = f^*$ and $L = \frac{1}{\mu}$. As ∇g is Lipschitz with constant L, so is $g_x(z) = g(z) - \nabla g(x)^T z$, hence

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$$\frac{1}{2L}\|\nabla g(x) - \nabla g(y)\|^2 \leq g(y) - g(x) + \nabla g(x)^T (x - y)$$

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Let $u = \nabla f(x)$, $v = \nabla g(y)$; then $x \in \partial g^*(u)$, $y \in \partial g^*(v)$, and the above reads $(x - y)^T (u - v) \geq \frac{\|u-v\|^2}{L}$, implying the result.

Conjugate function properties

Recall that given $f : \mathbb{R}^n \to \mathbb{R}$, the function defined by

$$f^*(y) = \max_x \left[y^T x - f(x) \right]$$

is called its conjugate.

- Conjugates appear frequently in dual programs, since

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- If f is strictly convex, then

$$\nabla f^*(y) = \arg\min_z \left[f(z) - y^T z \right]$$

Conjugate function properties (proofs)

We will show that $x \in \partial f^*(y) \Leftrightarrow y \in \partial f(x)$, assuming that f is convex and closed.

- **Proof of** $\Leftarrow$: Suppose $y \in \partial f(x)$. Then $x \in M_y$, the set of maximizers of $y^T z - f(z)$ over z. But

$$f^*(y) = \max_z \{y^T z - f(z)\} \quad \text{and} \quad \partial f^*(y) = \text{cl}(\text{conv}(\bigcup_{z \in M_y} \{z\})).$$

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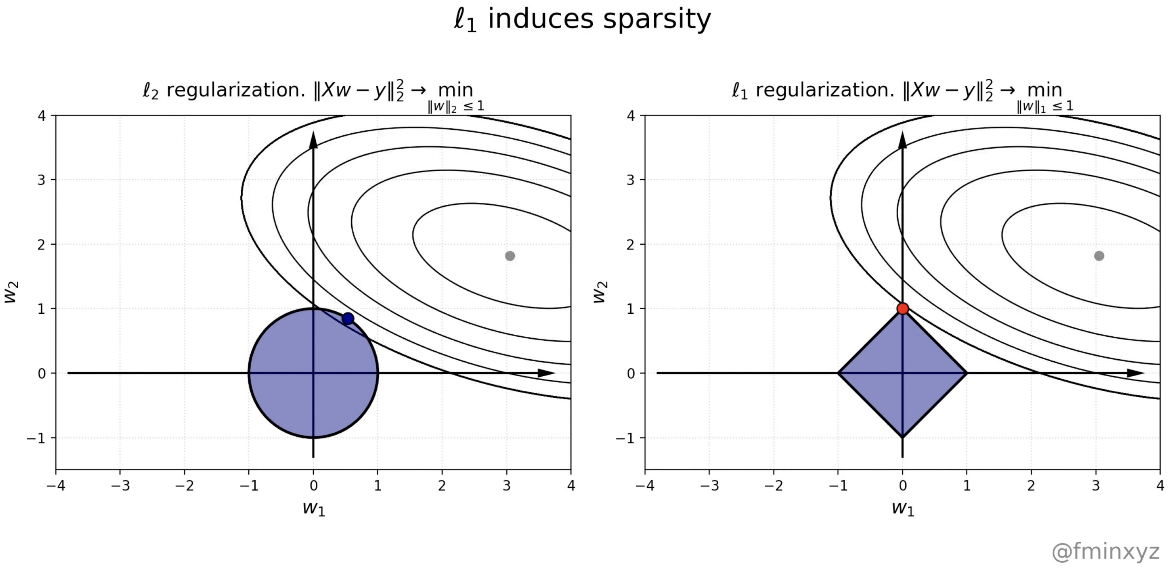
- **Proof of** $\Rightarrow$: From what we showed above, if $x \in \partial f^*(y)$, then $y \in \partial f^*(x)$, but $f^{**} = f$.

Clearly $y \in \partial f(x) \Leftrightarrow x \in \arg\min_z \{f(z) - y^T z\}$

Lastly, if f is strictly convex, then we know that $f(z) - y^T z$ has a unique minimizer over z, and this must be $\nabla f^*(y)$.

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.

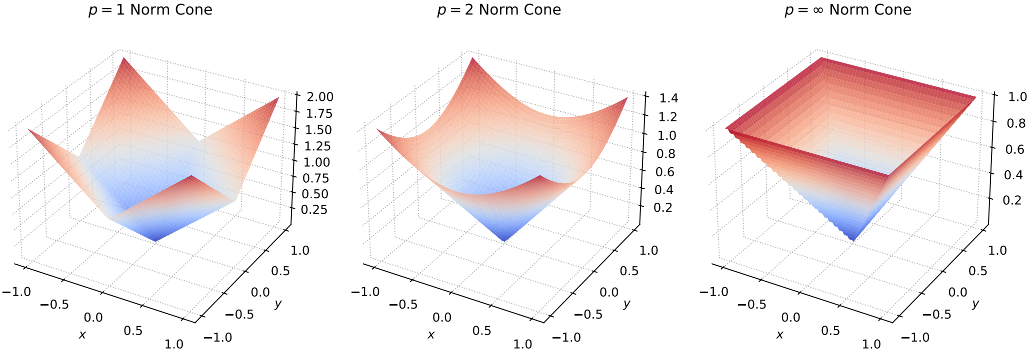


Figure 5: Norm cones for different p - norms are non-smooth

Convex function linear lower bound

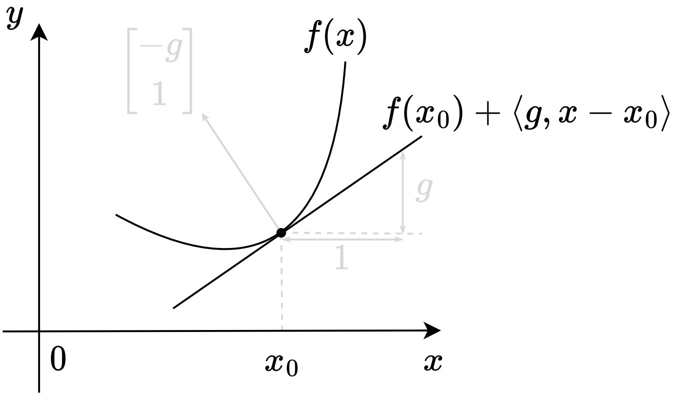


Figure 6: Taylor linear approximation serves as a global lower bound for a convex function

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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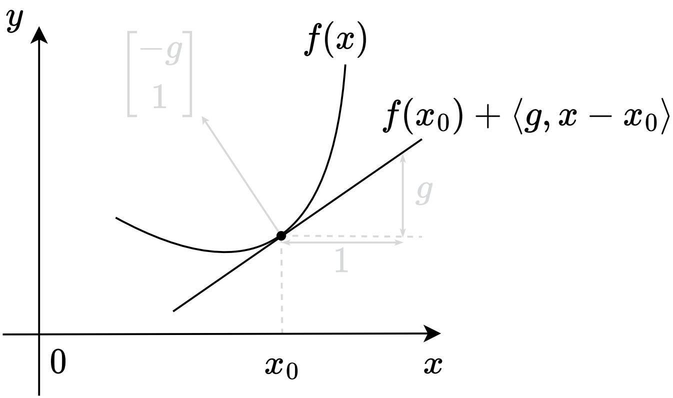

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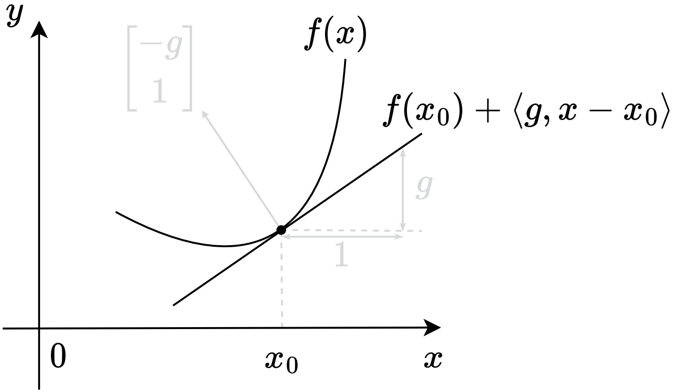

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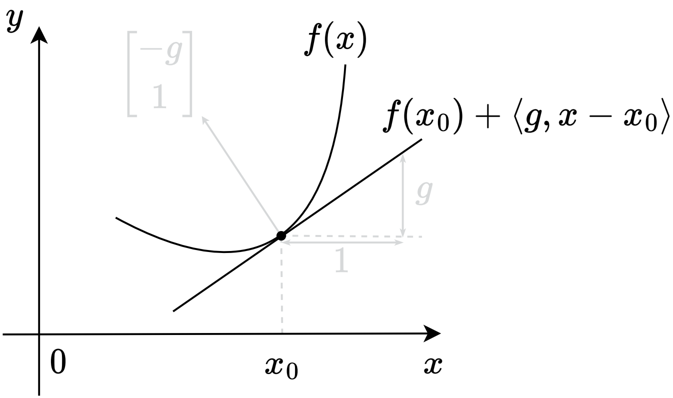
Convex function linear lower bound



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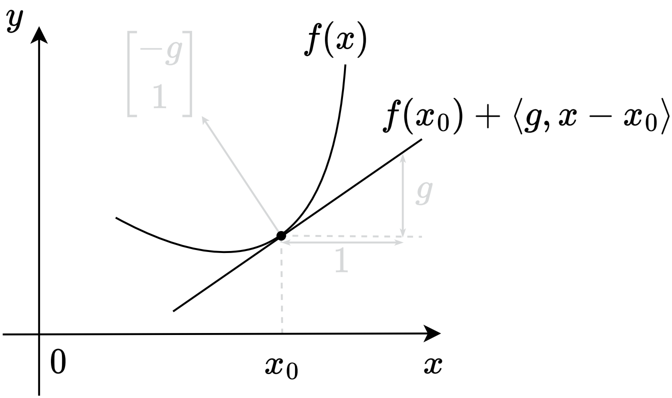

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We wouldn't want to lose such a nice property.

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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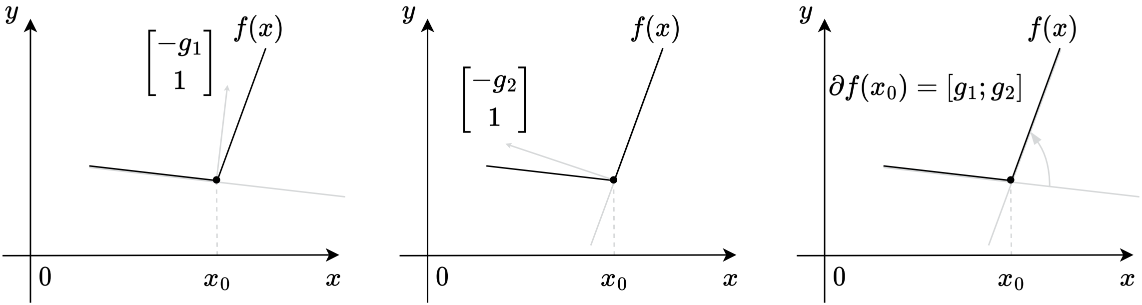

Figure 7: Subdifferential is a set of all possible subgradients

Subgradient and subdifferential

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

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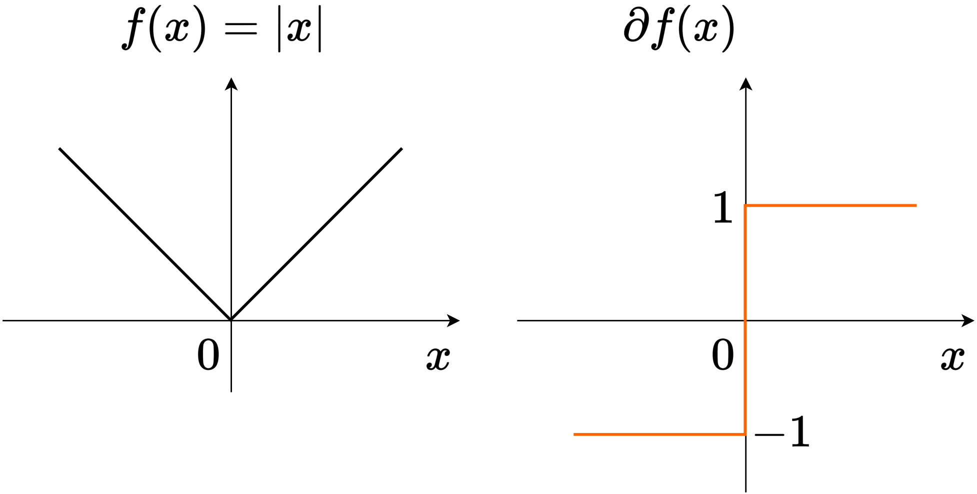

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Subdifferential of a differentiable function

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

$$f(x_0 + tv) \geq f(x_0) + t\langle s, v \rangle$$

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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

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

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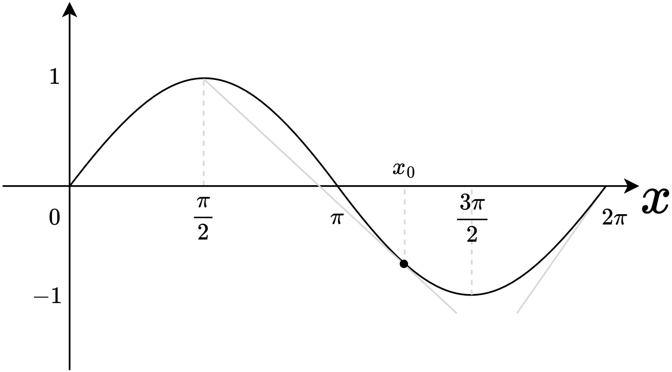
Find $\partial f(x)$, if $f(x) = \sin x, x \in [\pi/2; 2\pi]$



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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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- $\partial(f(Ax + b))(x) = A^T \partial f(Ax + b)$, f - convex function
- $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$.

Connection to convex geometry

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

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

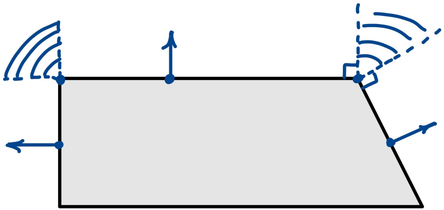
For $x \in S$, $\partial I_S(x) = \mathcal{N}_S(x)$, the **normal cone** of S at x is, recall

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

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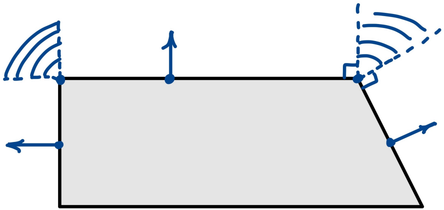
- For $y \in S$, this means $0 \geq g^T(y - x)$



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

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

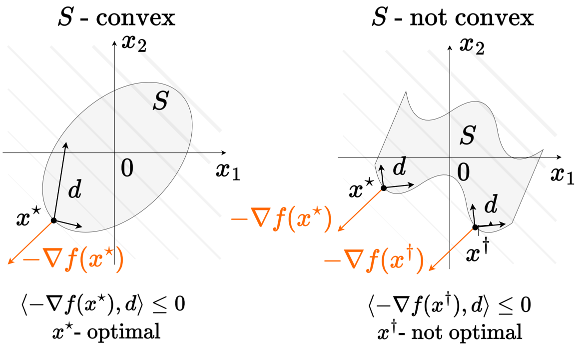
Intuitively: this says that the gradient increases as we move away from x. How to prove it? First, recast the problem as

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

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

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

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

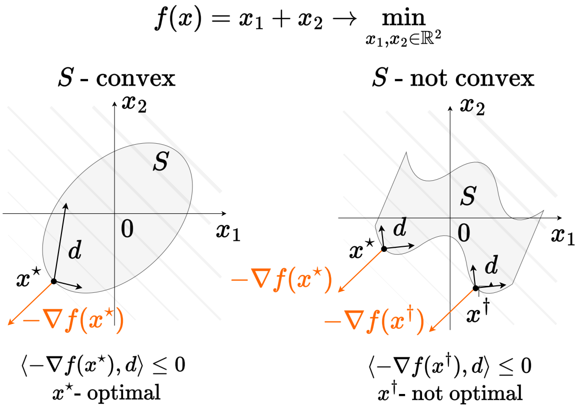
$$\Leftrightarrow -\nabla f(x) \in \mathcal{N}_S(x)$$

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

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

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).



Example 1

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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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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 $q \geq 1$. 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

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

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.