



Subgradient. Optimality conditions

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Optimization methods. MIPT

Subgradient and Subdifferential

ℓ_1 -regularized linear least squares

ℓ_1 induces sparsity

ℓ_2 regularization. $\|Xw - y\|_2^2 \rightarrow \min_{\|w\|_2 \leq 1}$



ℓ_1 regularization. $\|Xw - y\|_2^2 \rightarrow \min_{\|w\|_1 \leq 1}$



@fminxyz

Norms are not smooth

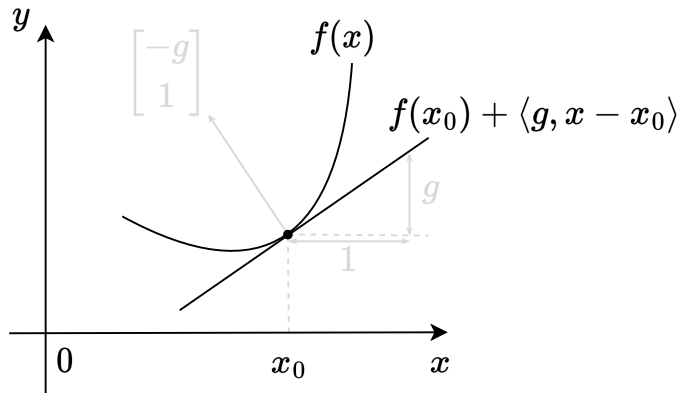
$$\min_{x \in \mathbb{R}^n} f(x),$$

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



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:

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

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

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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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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 $f(x) : S \rightarrow \mathbb{R}$ 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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Let $f : S \rightarrow \mathbb{R}$ be a function defined on the set S in a Euclidean space \mathbb{R}^n . If $x_0 \in \text{ri}(S)$ 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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for all $0 < t < \delta$. Taking the limit as t approaches 0 and using the definition of the gradient, we get:

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

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

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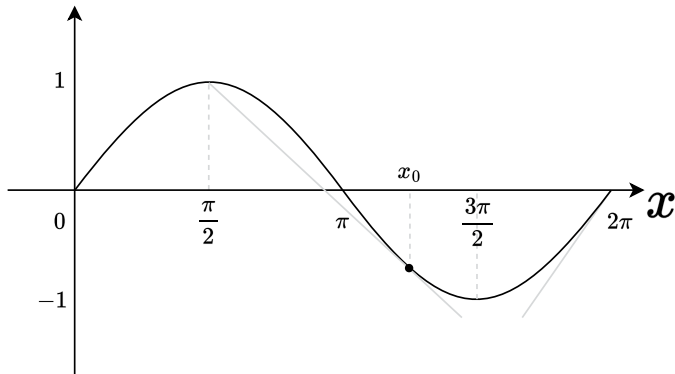
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Find $\partial f(x)$, if $f(x) = \sin x, x \in [\pi/2; 2\pi]$



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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 $f : [0, \infty) \rightarrow \mathbb{R}$ 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 $s \leq -\sqrt{1/x}$ for all $x > 0$. Taking the limit as x approaches 0 from the right, we get $s \leq -\infty$, which is impossible.

Subdifferential calculus

i 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 $\bigcap_{i=1}^n \text{ri}(S_i) \neq \emptyset$ 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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i 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 $f(x) = \max_i f_i(x)$. Then:

$$\partial_S f(x_0) = \text{conv} \left\{ \bigcup_{i \in I(x_0)} \partial_S f_i(x_0) \right\}, \quad I(x) = \{i \in [1, n] \mid f_i(x) = f(x)\}$$

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- $z \in \partial f(x)$ if and only if $x \in \partial f^*(z)$.
- Let $f : E \rightarrow \mathbb{R}$ be a convex function and $g : \mathbb{R} \rightarrow \mathbb{R}$ 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 $I_S : \mathbb{R}^n \rightarrow \mathbb{R}$,

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

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



Optimality Condition

For any f (convex or not),

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

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

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

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

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:

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

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



$$\langle -\nabla f(x^*), d \rangle \leq 0$$

x^* - optimal



$$\langle -\nabla f(x^\dagger), d \rangle \leq 0$$

x^\dagger - not optimal

Derivation of first-order optimality

Observe

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

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

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

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

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

as desired.

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

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

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

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

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

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

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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.

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

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

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



Figure 5: Illustration of different stationary (critical) points

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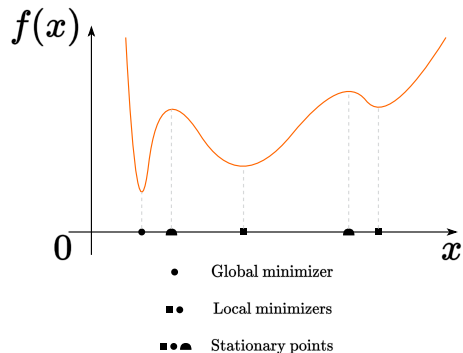


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- We call x^* a **stationary point** (or critical) if $\nabla f(x^*) = 0$. Any local minimizer of a differentiable function must be a stationary point.

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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Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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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$$\nabla f(x^*) = 0$$

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Because ∇f is continuous near x^* , there is a scalar $T > 0$ such that 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.

$$p^T \nabla f(x^* + tp) < 0, \text{ for all } t \in [0, T]$$

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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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Non-convex PL function



Constrained optimization

General first-order local optimality condition

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Figure 7: General first order local optimality condition

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- If $f(x)$ - strictly or strongly convex function, then S^* contains only one single point $S^* = \{x^*\}$.

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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 $h(x) = x_1^2 + x_2^2 - 2$.

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We want: $f(x_F + \delta x) \leq f(x_F)$



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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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$$\nabla_\nu L(x^*, \nu^*) = 0 \text{ budget constraint}$$

Sufficient conditions

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

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

Lagrangian

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

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

Then if the problem is *regular* (we will define it later) and the point x^* is the local minimum of the problem described above, then there exists ν^* :

Necessary conditions

$$\nabla_x L(x^*, \nu^*) = 0 \text{ that's written above}$$

$$\nabla_\nu L(x^*, \nu^*) = 0 \text{ budget constraint}$$

Sufficient conditions

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

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

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

Equality constrained problem

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

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

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

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

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

Linear Least Squares

i 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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- $m = n$
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