## EN.553.741: Machine Learning

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## 1.1 Unconstrained Optimization

In unconstrained optimization problem, we minimize an objective function  $f: \mathbb{R}^d \to \overline{\mathbb{R}}$  depending on a variable  $x \in \mathbb{R}^d$  without restrictions on x. The mathematical formulation is

$$\underset{x \in \mathbb{R}^d}{\text{minimize } f(x).} \tag{1.1}$$

We are only interested in those functions f which are bounded below, otherwise the minimum of f is  $-\infty$ .

**Definition 1.1.** A point  $x^* \in \mathbb{R}^d$  is called a **global minimizer** if  $f(x^*) \leq f(x)$  for all  $x \in \mathbb{R}^d$ . A point  $x^*$  is a **local minimizer** if there is a neighborhood U of  $x^*$  such that  $f(x^*) \leq f(x)$  for all  $x \in U$ .

Even if a function is bounded below, the global minimizer may not exist, e.g., the function  $f(x) = e^x$  for  $x \in \mathbb{R}$  is bounded below, since it is nonnegative. However, the infimum of f is 0 which cannot be attained by any  $x \in \mathbb{R}$ . The global minimizer is usually difficult to find, because our knowledge of f is usually only local. Most algorithms in practice only aim at finding local minimizer.

**Definition 1.2.** A point  $x^*$  is a **strict local minimizer** if there is a neighborhood U of  $x^*$  such that  $f(x^*) < f(x)$  for all  $x \in U \setminus \{x^*\}$ . A point  $x^*$  is an **isolated local minimizer** if there is a neighborhood U of  $x^*$  such that  $x^*$  is the only minimizer in U.

The strict local minimizer are not necessarily isolated, e.g., the function f defined by

$$f(x) \coloneqq \begin{cases} x^4 \cos(1/x) + 2x^4 & \text{if } x \neq 0; \\ 0 & \text{if } x = 0 \end{cases}$$

is of class  $C^2(\mathbb{R})$  and has a strict local minimizer at  $x^* = 0$ . And there are strict local minimizers at many points of  $x_j$ , these points are labeled such that  $x_j \downarrow 0$  as  $j \to \infty$ . However, it is easy to see that all isolated local minimizers are strict.

If the function f is sufficiently smooth, we can exploit its gradient and Hessian to tell whether or not  $x^*$  is a local minimizer.

**Theorem 1.3.** Let  $f \in C^1(\mathbb{R}^d)$  and  $p \in \mathbb{R}^d$ . Then we have

$$f(x+p) = f(x) + \nabla f(x+tp)^{\mathsf{T}} p \tag{1.2}$$

for some  $t \in (0,1)$ . Moreover, if  $f \in C^2(\mathbb{R}^d)$ , we have that

$$\nabla f(x+p) = \nabla f(x) + \int_0^1 \nabla^2 f(x+tp)p, \qquad (1.3)$$

and that

$$f(x+p) = f(x) + \nabla f(x)^{\mathsf{T}} p + \frac{1}{2} p^{\mathsf{T}} \nabla^2 f(x+tp) p,$$
 (1.4)

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

Necessary conditions for optimality are derived by assuming that  $x^*$  is a local minimizer and then proving facts about  $\nabla f(x^*)$  and  $\nabla^2 f(x^*)$ .

**Theorem 1.4** (First-order Necessary Conditions). If  $x^*$  is a local minimizer and f is continuously differentiable in an open neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$ .

**Theorem 1.5** (Second-order Necessary Conditions). If  $x^*$  is a local minimizer of f, and  $\nabla^2 f$  exists and is continuous in an open neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive semidefinite.

The necessary conditions in Theorem 1.5 are not sufficient. For example, let  $f(x) = x^3$ , then f'(0) = 0 and f''(0) = 0. But f is not a local minimizer at x = 0. We now describe sufficient conditions under which  $x^*$  is a local minimizer.

**Theorem 1.6.** Suppose that  $\nabla^2 f$  exists and is continuous in an open neighborhood of  $x^*$ , and that  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive definite. Then  $x^*$  is a strict local minimizer of f.

Note too that the second-order sufficient conditions are not necessary: A point  $x^*$  may be a strict local minimizer, and may fail to satisfy the sufficient conditions. A simple example is given by the function  $f(x) = x^4$ , for which the point  $x^* = 0$  is a strict local minimizer at which the Hessian vanishes.

All algorithms for unconstrained optimization problem require the user to supply a initial point, which is usually denoted by  $x_0$ . Beginning at  $x_0$ , the optimization algorithms generate a sequence of iterates  $(x_k)_{k \in \mathbb{N}_0}$  that terminate when

- no more progress can be made;
- a solution has been approximated with sufficient accuracy.

## 1.2 Convex Analysis

Our aim is to introduce basic concepts in convex analysis. The space V is a normed vector space equipped with norm  $\|\cdot\|$  unless otherwise specified.

**Definition 1.7.** A subset  $\Omega$  of V is called **convex** if

$$\alpha x + (1 - \alpha)y \in \Omega$$

for all  $x, y \in \Omega$  and  $\alpha \in [0, 1]$ .

The empty set is by convention considered to be convex. The following proposition gives some operations that preserve convexity of a set.

**Proposition 1.8.** 1. Let I be an arbitrary index set. If  $(A_i)_{i \in I}$  is a sequence of convex sets, then  $\bigcap_{i \in I} A_i$  is still a convex set.

- 2. The vector same  $A_1 + A_2 = \{x + y : x \in A_1, y \in A_2\}$  is a convex set provided  $A_1, A_2$  are both convex.
- 3. The scalar multiple of a convex set  $\alpha A = \{\alpha x : x \in A\}$  is convex. Moreover we have the set equation

$$\alpha_1 A + \alpha_2 A = (\alpha_1 + \alpha_2) A$$

where  $\alpha_1, \alpha_2 \in [0, +\infty)$ .

- 4. The closure and the interior of a convex set are convex.
- 5. The image and the inverse image of a convex set under an affine function are convex.

If a is a nonzero vector in  $V = \mathbb{R}^d$  and  $b \in \mathbb{R}$ , then we have the following definition. A **hyperplane** is a set specified by a set of the form  $\{x: a^{\mathsf{T}}x = b\}$ . A **halfspace** is a set specified by a set of the form  $\{x: a^{\mathsf{T}}x \leq b\}$ . It is clearly closed and convex. A set is said to be **polyhedral** if it is nonempty and it is the intersection of a finite number of halfspaces. A polyhedral set is convex and closed, being the intersection of halfspaces. A set A is said to be a **cone** if for all

 $x \in A$  and  $\alpha > 0$ , we have  $\alpha x \in A$ . A cone may not be convex and may not contain the origin, although the origin always lies in the closure of a non-empty cone. A **polyhedral cone** is a set of the form

$$\bigcap_{i=1}^{n} \left\{ x : a_i^\mathsf{T} x \le 0 \right\}$$

where  $a_1, ..., a_n \in \mathbb{R}^d$ . A subspace is a special case of a polyhedral cone, which is in turn a special case of a polyhedral set.

**Definition 1.9.** Let  $\Omega$  be a convex subset of V. A function  $f: \Omega \to (-\infty, +\infty)$  is called **convex** if

$$f(\alpha x + (1 - \alpha)y)) \le \alpha f(x) + (1 - \alpha)f(y)$$

for all  $x, y \in \Omega$  and  $\alpha \in [0,1]$ . A function f is called strictly convex if the inequality above is strict. A function f is **concave** if -f is convex.

Common examples of convex functions are affine functions and  $\|\cdot\|$ , etc. If  $f:\Omega\to\mathbb{R}$  is a function and  $\lambda\in\mathbb{R}$  is a scalar, the sets  $\{x\in\Omega:f(x)\leq\lambda\}$  and  $\{x\in\Omega:f(x)<\lambda\}$  are called the **level sets** of f. If  $x,y\in\Omega$  with  $f(x)\leq\lambda$  and  $f(y)\leq\lambda$  for some convex function f, then for every  $\alpha\in[0,1]$ , we have

$$f(\alpha x + (1 - \alpha)y) \le \alpha f(x) + (1 - \alpha)f(y) \le \lambda$$

by the convexity of f. So the level sets for convex functions are convex. However the converse is not true as illustrated in the following example.

**Example 1.10.**  $f(x) = \sqrt{|x|}$  is not a convex function, and  $\{x : f(x) \le \lambda\} = \{x : |x| \le \lambda^2\}$  is convex for sure.

In the context of optimization and duality, we will encounter operations resulting functions taking infinite values. For example, the supremum of a infinite collection of functions. We thus are motivated to consider *extended real-valued* functions that can take the values  $\pm \infty$  at some points. Such functions can be characterized using the notion of epigraph discussed below.

**Definition 1.11.** The **epigraph** of a function  $f: \Omega \to [-\infty, +\infty]$ , where  $\Omega$  is a subset of V, is defined to be a subset of  $V \times \mathbb{R}$  given by

$$epi(f) = \{(x, y) : x \in \Omega, y \in \mathbb{R}, f(x) \le y\}$$

the effective domain of f is defined to be the set

$$dom(f) = \{x \in \Omega : f(x) < +\infty\}$$
(1.5)

We say that f is **proper** if  $f(x) < +\infty$  for at least one  $x \in \Omega$ , i.e. ,  $dom(f) \neq \emptyset$ , and  $f(x) > -\infty$  for all  $x \in \Omega$ , i.e. , epi(f) does not contain a vertical line, we call f is **improper** otherwise.

In order to avoid  $\infty - \infty$  in the definition for an improper convex function, it is convenient to define convex extended real-valued function by its epigraph

**Definition 1.12.** Let  $\Omega$  be a convex subset of V. We say that an extended real-valued function  $f: \Omega \to [-\infty, +\infty]$  is convex if  $\operatorname{epi}(f)$  is a convex subset of  $V \times \mathbb{R}$ .

It can be easily shown that, according to Definition 1.12, convexity of f implies that its effective domain dom(f) and its level sets

$$\{x \in \Omega : f(x) \le \lambda\}, \quad \{x \in \Omega : f(x) < \lambda\}$$

are convex sets for all scalars  $\lambda \in \mathbb{R}$ .

Exercise 1.13. Prove the assertions above.

Definition 1.12 is consistent with the earlier definition of convexity for real-valued functions.

**Exercise 1.14.** If  $f(x) < \infty$  for all  $x \in \Omega$ , or  $f(x) > -\infty$  for all  $x \in \Omega$ , then

$$f(\alpha x + (1 - \alpha)y) \le \alpha f(x) + (1 - \alpha)f(y)$$

for all  $x, y \in \Omega$  and  $\alpha \in [0, 1]$ . In particular, Definition 1.12 is consistent with Definition 1.9.

By passing to epigraphs, we can use results about sets to infer corresponding results about functions. The reverse is also possible, via function  $\delta_{\Omega}: V \to (-\infty, +\infty]$  of a set  $\Omega \subset V$ , defined by

$$\delta_{\Omega}(x) = \begin{cases} 0 & \text{if } x \in \Omega \\ \infty & \text{otherwise.} \end{cases}$$
 (1.6)

A set A is convex if and only if  $\delta_A$  is a convex function, and A is nonempty if and only if  $\delta_A$  is proper. If the epigraph of a function  $f: \Omega \to [-\infty, +\infty]$  is a closed set, we say that f is a **closed function**. Closedness is related to the classical notion of lower semi-continuity.

**Definition 1.15.** An extended real-valued function f is called **lower semicontinuous** at a  $x \in \Omega$  if

$$f(x) \le \liminf_{k \to \infty} f(x_k)$$

for every sequence  $\{x_k\}_{k=1}^{\infty} \subset \Omega$  with  $x_k \to x$ . We say that f is **upper semicontinuous** if -f is lower semicontinuous.

The following proposition connects closedness, lower semicontinuity, and closedness of the level sets of a function.

**Proposition 1.16.** For an extended real-valued function  $f: V \to [-\infty, +\infty]$ , the following are equivalent

- 1. The level set  $\{x: f(x) \leq \lambda\}$  is closed for every  $\lambda \in \mathbb{R}$ .
- 2. f is lower semicontinuous.
- 3. epi(f) is a closed set.

**Corollary 1.17.** The level set  $\{x: f(x) < \lambda\}$  is open for every  $\lambda \in \mathbb{R}$  if and only if f is upper semicontinuous.

In practice, we prefer to use the closeness notion, rather than lower semicontinuity. One reason is that contrary to closeness, lower semicontinuity is a domain dependent property. For example  $\delta_{(0,1)}$  is neither closed or lower semicontinuous on  $V = \mathbb{R}$ ; but if its domain is restricted to (0,1) it becomes lower semicontinuous.

The local minimum of a convex function is also a global minimum.

**Theorem 1.18.** If  $\Omega$  is a convex subset of V and  $f:V \to (-\infty,\infty]$  is a convex function, then a local minimum of f over  $\Omega$  is also a global minimum. If f is strictly convex, then there exists at most one global minimum of f over  $\Omega$ .