INFR10086 Machine Learning (MLG) Semester 2, 2023/4

Optimization 1

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Definition 1. The minimum of a function $f : \mathbb{R}^d \to \mathbb{R}$ is written as $\min_x f(x)$, and has the property that $\min_x f(x) \le f(y)$ for any y.

Definition 2. The value x^* such that $f(x^*) = \min_x f(x)$ is called a minimizer.

Example 1. For the parabola $f(x) = x^2 + 4x - 1 = (x + 2)^2 - 5$, the minimum is -5 and the mimimizer is $x = -2$.

Definition 3. A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if for any $0 \le \alpha \le 1$, we have

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

for any x and y.

Definition 4. A function f is concave if $-f$ is convex.

Example 2. If f is convex, then

$$f(x) \ge f(y) + \nabla f(y)^\top (x - y) \tag{2}$$

for any x and y.

We can arrenge the following

$$f(\alpha x + (1 - \alpha)y) \le \alpha f(x) + (1 - \alpha)f(y) \tag{3}$$

into

$$f(y) + \frac{f(y + \alpha(x - y)) - f(y)}{\alpha} \le f(x). \tag{4}$$

Remember that this holds for any $0 \le \alpha \le 1$. In particular, if we take the limit,

$$f(y) + \lim_{\alpha \to 0} \frac{f(y + \alpha(x - y)) - f(y)}{\alpha} = f(y) + \nabla f(y)^\top (x - y) \le f(x). \tag{5}$$

Definition 5. A matrix A is positive semidefinite if $v^\top Av \geq 0$ for all v, and is written as $A \succeq 0$.

Example 3. A function is convex if its Hessian is positive semidefinite.

The proof relies on mean-value theorem. It's not difficult, but is beyond the scope of this course.

Example 4. Show that the mean-squared error $\ell(y, \hat{y}) = (y - \hat{y})^2$ is convex in $\hat{y}$.

$$\frac{\partial^2}{\partial \hat{y}^2}\ell = 2 \geq 0. \tag{6}$$

Example 5. Show that the function

$$f(x) = x^\top \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} x \tag{7}$$

is convex.

The Hessian of f is $\begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}$. For any $v = \begin{bmatrix} v_1 & v_2 \end{bmatrix}^\top$, we have

$$\begin{bmatrix} v_1 & v_2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 2v_1 & 3v_2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = 2v_1^2 + 3v_2^2 \geq 0 \tag{8}$$

The Hessian of f is positive semidefinite.

Example 6. Show that the Hessian of $f(x) = \|x\|_2^2$ is $2I$, and hence $\|x\|_2^2$ is convex in x.

$$\frac{\partial^2}{\partial x_i \partial x_j} f = 0 \qquad \frac{\partial^2}{\partial x_i^2} f = 2 \tag{9}$$

Example 7. Show that if f is convex, then $g(x) = f(Ax + b)$ is also convex.

$$g(\alpha x + (1 - \alpha)y) = f(\alpha(Ax + b) + (1 - \alpha)(Ay + b)) \tag{10}$$

$$\leq \alpha f(Ax + b) + (1 - \alpha)f(Ay + b) = \alpha g(x) + (1 - \alpha)g(y) \tag{11}$$

Example 8. Show that if $f_1, \ldots, f_k$ are convex, then $f = \beta_1 f_1 + \cdots + \beta_k f_k$ is also convex when $\beta_1, \ldots, \beta_k \geq 0$.

$$
\begin{aligned}
f(\alpha x + (1-\alpha)y) &= \beta_1 f_1(\alpha x + (1-\alpha)y) + \cdots + \beta_k f_k(\alpha x + (1-\alpha)y) &(12)\\
&\leq \beta_1 \alpha_1 f_1(x) + \beta_1(1-\alpha) f_1(y) + \cdots + \beta_k \alpha f_k(x) + \beta_k (1-\alpha) f_k(y) &(13)\\
&= \alpha(\beta_1 f_1(x) + \cdots + \beta_k f_k(x)) + (1-\alpha)(\beta_1 f_1(y) + \cdots + \beta_k f_k(y)) &(14)\\
&= \alpha f(x) + (1-\alpha) f(y) &(15)
\end{aligned}
$$

Exercise 1. Given a data set of n samples $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, show that

$$L = \sum_{i=1}^{n} (w^\top x_i - y_i)^2 = \|Xw - y\|_2^2 \tag{16}$$

if we have

$$X = \begin{bmatrix} - & x_1 & - \\ & \vdots & \\ - & x_n & - \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}. \tag{17}$$

Exercise 2. Given a data set of n samples $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, show that the mean-squared error

$$L = \|Xw - y\|_2^2 \tag{18}$$

is convex.

Example 9. Show that if f is convex and $\nabla f(x^*) = 0$ for a point x^*, then x^* is the minimizer of f.

Because f is convex, we have for any x and y,

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y). \tag{19}$$

In particular, if we let $y = x^*$,

$$f(x) \geq f(x^*) + \nabla f(x^*)^\top (x - x^*) = f(x^*). \tag{20}$$

Example 10. Show that $\nabla_x (x^\top A x) = (A^\top + A)x$.

We see that $x^\top A x$ is a real value. If we take the derivative of $x^\top A x$, we get

$$
\begin{aligned}
\frac{\partial}{\partial x_k} \sum_{i=1}^{d} \sum_{j=1}^{d} a_{ij} x_i x_j &= \sum_{i \neq j}^{d} a_{ik} x_i + \sum_{j \neq i}^{d} a_{kj} x_j + \sum_{i=1}^{d} 2 a_{ii} x_i &(21)\\
&= \sum_{i=1}^{d} a_{ik} x_i + \sum_{j=1}^{d} a_{kj} x_j = a_{\cdot k}^\top x + a_{k\cdot} x &(22)
\end{aligned}
$$

where $a_{\cdot k}$ is the k-th column of A and $a_{k\cdot}$ is the k-th row of A.

Example 11. Show that $w^* = (X^\top X)^{-1} X^\top y$ is the minimizer for $L = \|Xw - y\|_2^2$.

$$L = (Xw - y)^\top (Xw - y) = w^\top X^\top X w - 2y^\top X w + y^\top y \tag{23}$$

$$\nabla L = (X^\top X + X^\top X) w - 2X^\top y = 0 \tag{24}$$

If $w^* = (X^\top X)^{-1} X^\top y$, then $\nabla L(w^*) = 0$. Because L is convex in w, w^* is a minimizer of L.

Example 12. Show that $\ell(s) = \log(1 + \exp(-s))$ is convex in s.

$$\frac{\partial \ell}{\partial s} = \frac{-\exp(-s)}{1 + \exp(-s)} = \frac{1}{1 + \exp(-s)} - 1 \tag{25}$$

$$\frac{\partial^2 \ell}{\partial s^2} = \frac{-1}{1 + \exp(-s)} \frac{-\exp(-s)}{1 + \exp(-s)} = \frac{1}{1 + \exp(-s)} \left(1 - \frac{1}{1 + \exp(-s)}\right) \geq 0 \tag{26}$$

Exercise 3. Given a data set of n samples $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, show that the log loss

$$L = \sum_{i=1}^{n} \log\left(1 + \exp(-y_i w^\top x_i)\right) \tag{27}$$

is convex.

Definition 6. A function $f : \mathbb{R}^d \to \mathbb{R}$ is called stricly convex if for $0 \leq \alpha \leq y$, we have

$$f(\alpha x + (1 - \alpha) y) < \alpha f(x) + (1 - \alpha) f(y) \tag{28}$$

for any $x \neq y$.

Exercise 4. A function $f : \mathbb{R}^d \to \mathbb{R}$ is stricly convex if

$$f(x) > f(y) + \nabla f(y)^\top (x - y) \tag{29}$$

for any $x \neq y$.

Definition 7. A matrix A is positive definite if $v^\top A v > 0$ for any $v \neq 0$.

Exercise 5. A function $f : \mathbb{R}^d \to \mathbb{R}$ is stricly convex if its Hessian is positive definite.

Example 13. Show that if f is strictly convex, then f has a unique minimizer.

Suppose x^* is a minimizer of f, i.e., $\nabla f(x^*) = 0$. The inequality

$$f(x) > f(y) + \nabla f(y)^\top (x - y). \tag{30}$$

holds for any $x \neq y$. In particular, if we let $y = x^*$,

$$f(x) > f(x^*) + \nabla f(x^*)^\top (x - x^*) = f(x^*). \tag{31}$$