Chapter 5 Smoothness and convexity

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After discussing Bayesian model in Chapter 3, we made some simplification to get linear models, the easiest but important ones in machine learning. Now, we should take a break for some mathematical foundations, in order to introduce more complex model based on linear models.

This chapter corresponds to Chapter 1,3,4 of PRML, Chapter of UML. It mainly introduces some important properties regarding with functions: convexity, smoothness, strong convexity and Lipschitzness. And the next chapter will introduces some optimization techniques, which are the tools for solving machine learning models.

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1 Convexity

Definition 5.1 (convex set) A set C in a vector space is convex if for any two vectors \mathbf{u} , \mathbf{v} in C, the line segment between them is in C, that is, for any $\alpha \in [0,1]$, $\alpha \mathbf{u} + (1-\alpha)\mathbf{v} \in C$.

Definition 5.2 (convex function) Let C be a convex set. A function $f:C\to \mathcal{R}$ is convex if for all $\mathbf{u},\mathbf{v}\in C$ and $\alpha\in[0,1]$,

$$f(\alpha \mathbf{u} + (1 - \alpha)\mathbf{v}) \le \alpha f(\mathbf{u}) + (1 - \alpha)f(\mathbf{v})$$

Claim 5.1 local minimum of convex function is global minimum

Proof Let $B(\mathsf{u},r)=\{\mathsf{v}:\|\mathsf{v}-\mathsf{u}\|\leq r\}$, we say that $f(\mathsf{u})$ is a local minimum if there exists some r>0 such that $\forall \mathsf{v}\in B(\mathsf{u},r), f(\mathsf{v})\geq f(\mathsf{u})$. Then for any v (not necessarily in B), there exists a small enough $\alpha>0$ such that $\mathsf{u}+\alpha(\mathsf{v}-\mathsf{u})\in B(\mathsf{u},r)$, and therefore $f(\mathsf{u})\leq f(\mathsf{u}+\alpha(\mathsf{v}-\mathsf{u}))$. If f is convex, we also have $f(\mathsf{u}+\alpha(\mathsf{v}-\mathsf{u}))\leq (1-\alpha)f(\mathsf{u})+\alpha f(\mathsf{v})$, which leads to $f(\mathsf{u})\leq f(\mathsf{v})$ and hence is a global minimum.

Claim 5.2 For a convex function f, we can construct a tangent at any point that lies below the function everywhere. If f is differential, then we have

$$\forall \mathsf{u}, f(\mathsf{u}) \geq f(\mathsf{v}) + \nabla f(\mathsf{v})^{\top} (\mathsf{u} - \mathsf{v})$$

To generalize this inequality to non-differential functions, we should study for sub-gradient.

Definition 5.3 (sub-gradient) Define the sub-gradient of a function f at \mathbf{x} to be a vector $\mathbf{g} \in \mathcal{R}^d$ which satisfies that $f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{g}^\top(\mathbf{y} - \mathbf{x}), \forall \mathbf{y} \in \mathcal{R}^d$.

Theorem 5.1 Let f be a differential function, then f is convex iff. ∇f is monotonically non-decreasing, and iff. $\nabla^2 f$ is non-negative.

Ex1 $f(\mathbf{x}) = \mathbf{x}^{\top}\mathbf{x}$ is convex. To see this, note that $\nabla f(\mathbf{x}) = 2\mathbf{x}$ and $\nabla^2 f(\mathbf{x}) = 2$.

Ex2 Consider scalar function $f(x) = \log(1 + \exp(x))$. It is convex since $f'(x) = \frac{1}{1 + \exp(-x)}$, which is the sigmoid function, and $f''(x) = \frac{\exp(-x)}{(1 + \exp(-x))^2} > 0$.

Claim 5.1 (linear transformation preserves convexity) Assume that $g: \mathcal{R}^d \to \mathcal{R}$ can be written as $g(\mathbf{w}) = f(\mathbf{w}^\top \mathbf{x} + b)$, for some $\mathbf{x} \in \mathcal{R}^d$, $b \in \mathcal{R}$. Then, if f is convex, g is convex too.

Proof For $\mathbf{w}_1, \mathbf{w}_2 \in \mathcal{R}^d$, and $\alpha \in (0, 1)$

$$g(\alpha \mathbf{w}_1 + (1 - \alpha)\mathbf{w}_2) = f(\alpha \mathbf{w}_1^\top \mathbf{x} + (1 - \alpha)\mathbf{w}_2^\top \mathbf{x} + b)$$

$$= f(\alpha(\mathbf{w}_1^\top \mathbf{x} + b) + (1 - \alpha)(\mathbf{w}_2^\top \mathbf{x} + b))$$

$$\leq \alpha f(\mathbf{w}_1^\top \mathbf{x} + b) + (1 - \alpha)f(\mathbf{w}_2^\top \mathbf{x} + b) = \alpha g(\mathbf{x}_1) + (1 - \alpha)g(\mathbf{x}_2)$$

Following Claim5.1,

Ex3 $f(\mathbf{w}) = (\mathbf{w}^{\top}\mathbf{x} - b)^2$ is convex.

Ex4
$$f(\mathbf{w}) = \log(1 + \exp(-y\mathbf{w}^{\mathsf{T}}\mathbf{x}))$$
 is convex.

Claim 5.2 (Pointwise supremum of convex functions is convex) For $i=1,\cdots,r$, let $f_i:\mathcal{R}^d\to\mathcal{R}$ be a convex function, then $g(\mathbf{x})=\max_i f_i(\mathbf{x})$ is convex.

Proof For $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{R}^d$, and $\alpha \in (0, 1)$

$$\begin{split} g(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) &= \max_i f_i(\alpha \mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \max_i [\alpha f_i(\mathbf{x}_1) + (1-\alpha)f(\mathbf{x}_2)] \\ &\leq \alpha \max_i f_i(\mathbf{x}_1) + (1-\alpha) \max_i f_i(\mathbf{x}_2) = \alpha g(\mathbf{x}_1) + (1-\alpha)g(\mathbf{x}_2) \end{split}$$

Following Claim5.2,

Ex5 $g(\mathbf{x}) = |\mathbf{x}|$ is convex. Since $f_1(\mathbf{x}) = \mathbf{x}$, $f_2(\mathbf{x}) = -\mathbf{x}$ are both convex, and $g(\mathbf{x}) = \max\{f_1(\mathbf{x}), f_2(\mathbf{x})\}$.

Claim 5.3 (linear combination with non-negative weights preserves convexity) For $i=1,\cdots,r$, let $f_i:\mathcal{R}^d\to\mathcal{R}$ be a convex function, then $\forall w_i\geq 0, i\in[1,r], g(\mathbf{x})=\sum_i w_i f_i(\mathbf{x})$ is convex.

Proof For $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{R}^d$, and $\alpha \in (0,1)$

$$g(\alpha \mathbf{x}_{1} + (1 - \alpha)\mathbf{x}_{2}) = \sum_{i} w_{i} f_{i}(\alpha \mathbf{x}_{1} + (1 - \alpha)\mathbf{x}_{2}) \leq \sum_{i} w_{i}(\alpha f_{i}(\mathbf{x}_{1}) + (1 - \alpha)f(\mathbf{x}_{2}))$$

$$= \alpha \sum_{i} w_{i} f_{i}(\mathbf{x}_{1}) + (1 - \alpha) \sum_{i} w_{i} f(\mathbf{x}_{2}) = \alpha g(\mathbf{x}_{1}) + (1 - \alpha)g(\mathbf{x}_{2})$$

Theorem 5.2 Jensen's Inequality Let $f: \mathcal{R}^d \to \mathcal{R}$ be a measurable convex function and $x \in \mathcal{R}^d$, $\mathbb{E}[\S]$ exists. Then

$$\mathbb{E}[f(\mathbf{x})] \ge f(\mathbb{E}[\mathbf{x}])$$

Ex6 Consider function f(x) = |x|, then the sub-differential set $\partial f(x)$ is

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

Ex7 Sub-gradient of Hinge loss. Consider the loss $l(x) = \max(1 - \mathbf{z}^{\top}\mathbf{x}, 0)$, then the sub-differential set is

$$\partial f(x) \left\{ \begin{aligned} \{\mathbf{0}\}, \ 1 - \mathbf{z}^{\top} \mathbf{x} < 0 \\ \{-\alpha \mathbf{z}, \alpha \in [0, 1]\}, \ 1 - \mathbf{z}^{\top} \mathbf{x} = 0 \\ \{-\mathbf{z}\}, \ 1 - \mathbf{z}^{\top} \mathbf{x} > 0 \end{aligned} \right.$$

2 Strong convexity

Definition 5.5 (strongly convex function) A function f is λ -strongly convex if for all $u, v \in C$ and $\alpha \in [0, 1]$,

$$f(\alpha \mathbf{u} + (1 - \alpha)\mathbf{v}) \le \alpha f(\mathbf{u}) + (1 - \alpha)f(\mathbf{v}) - \frac{\lambda}{2}\alpha(1 - \alpha)\|\mathbf{u} - \mathbf{v}\|_2^2$$

Theorem 5.3 If f is λ -strongly convex then for every \mathbf{u}, \mathbf{v} and $\mathbf{g} \in \partial f(\mathbf{v})$ we have

$$f(\mathbf{v}) \geq f(\mathbf{u}) + \mathbf{g}^{ op}(\mathbf{u} - \mathbf{v}) + rac{\lambda}{2} \|\mathbf{u} - \mathbf{v}\|_2^2$$

Proof According to the definition,

$$\begin{split} f(\mathbf{u}) &\geq \frac{f(\alpha \mathbf{u} + (1-\alpha)\mathbf{v})}{\alpha} - \frac{1-\alpha}{\alpha} f(\mathbf{v}) + \frac{\lambda}{2} (1-\alpha) \|\mathbf{u} - \mathbf{v}\|_2^2 \\ &\geq \frac{f(\mathbf{v}) + \mathbf{g}^\top (\alpha \mathbf{u} + (1-\alpha)\mathbf{v}) - \mathbf{v})}{\alpha} - \frac{1-\alpha}{\alpha} f(\mathbf{v}) + \frac{\lambda}{2} (1-\alpha) \|\mathbf{u} - \mathbf{v}\|_2^2 \qquad \textit{(Claim 5.2)} \\ &= \frac{f(\mathbf{v}) + \alpha \mathbf{g}^\top (\mathbf{u} - \mathbf{v})}{\alpha} - \frac{1-\alpha}{\alpha} f(\mathbf{v}) + \frac{\lambda}{2} (1-\alpha) \|\mathbf{u} - \mathbf{v}\|_2^2 \\ &= f(\mathbf{v}) + \mathbf{g}^\top (\mathbf{u} - \mathbf{v}) + \frac{\lambda}{2} (1-\alpha) \|\mathbf{u} - \mathbf{v}\|_2^2 \end{split}$$

Note that it holds for all $\alpha \in [0,1]$, setting $\alpha = 0$ leads to the conclusion.

Corollary 5.1 If f is λ -strongly convex and \mathbf{v} is a minimizer of f, then for any \mathbf{u} , $f(\mathbf{v}) \geq f(\mathbf{u}) + \frac{\lambda}{2} \|\mathbf{u} - \mathbf{v}\|_2^2$.

Ex8 $f(\mathbf{x}) = \|\mathbf{x}\|_2^2$ is 2-strongly convex, $f(\mathbf{x}) = \lambda \|\mathbf{x}\|_2^2$ is 2λ -strongly convex. Note that $f(\mathbf{x}') = \lambda \|\mathbf{x}' - \mathbf{x} + \mathbf{x}\|_2^2 = \lambda \|\mathbf{x}\|_2^2 + 2\lambda \mathbf{x}^\top (\mathbf{x}' - \mathbf{x}) + \lambda \|\mathbf{x}' - \mathbf{x}\|_2^2$, in which $2\lambda \mathbf{x}$ is the gradient of $f(\mathbf{x})$.

Claim 5.4 If f is λ -strongly convex and g is convex, then f+g is λ -strongly convex.

Following Claim 5.4, if we will to optimize a convex loss function, then with l_2 -norm regularization, the loss function becomes strongly convex. This speeds up the convergence of learning procedure, which we will see in the next chapter.

3 Lipschitzness

Definition 5.6 (dual norm)

One way to understand 'dual norm' is that it is a way to measure how "big" are linear functionals. For example, consider the linear function f, we want to try to understand how big it is. So, we can measure 1 that is we measure how big is the output of the linear functional compared to its input x, where x is measured with some norm. Now, you can show that the above is equivalent to the dual norm of x. The definition of dual norm immediately implies $\mathbf{w}^{\top}\mathbf{x} \leq \|\mathbf{w}\|_{*}\|\mathbf{x}\|$.

Ex9 Dual norm of l_2 -norm is itself.

Definition 5.7 (Lipschitzness) A function $f: \mathcal{R}^d \to \mathcal{R}^k$ is ρ -Lipschitz over set C if for every $\mathbf{w}_1, \mathbf{w}_2 \in C$, $\|f(\mathbf{w}_1) - f(\mathbf{w}_2)\|_* \le \rho \|\mathbf{w}_1 - \mathbf{w}_2\|$.

In this chapter, we just focus on l_2 -norm. According to the mean value theorem, we have $f(\mathbf{w}_1) - f(\mathbf{w}_2) = g^{\top}(\mathbf{w}_1 - \mathbf{w}_2)$, where $\mathbf{g} \in \partial f(\mathbf{u})$, \mathbf{u} is some point between \mathbf{w}_1 and \mathbf{w}_2 . This leads to the following theorem.

Theorem 5.4 If f is Lipschitz w.r.t l_2 -norm, iff. for all $g \in \partial f(x)$, we have $\|g\|_2 \leq \rho$.

- Ex10 The function f(x) = |x| is 1-Lipschitz over \mathcal{R} , since $|x_1| |x_2| = |x_1 x_2 + x_2| |x_2| \le |x_1 x_2| + |x_2| |x_2| = |x_1 x_2|$.
- Ex11 The function $f(x) = \log(1 + \exp(x))$ is 1-Lipschitz over \mathcal{R} , since $|f'(x)| = |\frac{1}{1 + \exp(-x)}| \le 1$.
- Ex12 The function $f(x)=x^2$ is not ρ -Lipschitz over $\mathcal R$ for any ρ . However, over the set $C=\{x:|x|\leq \frac{\rho}{2}\}$, this function is ρ -Lipschitz. Indeed, for any $x_1,x_2\in C$, $|x_1^2-x_2^2|=|x_1+x_2||x_1-x_2|\leq 2\cdot \frac{\rho}{2}\cdot |x_1-x_2|=\rho|x_1-x_2|$.
- Ex13 Linear function $f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b$ is $\|\mathbf{w}\|$ -Lipschitz following Cauchy-Schwartz inequality $|f(\mathbf{x}_1) f(\mathbf{x}_2)| = |\mathbf{w}^{\top} (\mathbf{x}_1 \mathbf{x}_2)| \le \|\mathbf{w}\|_2 \|\mathbf{x}_1 \mathbf{x}_2\|_2$.

Claim 5.5 (Lipschitzness preserves on compound functions) Let $f(\mathbf{x}) = g_1(g_2(\mathbf{x}))$, where g_1 is ρ_1 -Lipschitz and g_2 is ρ_2 -Lipschitz. Then, f is $(\rho_1\rho_2)$ -Lipschitz. In particular, if g_2 is the linear function, $g_2(\mathbf{x}) = \mathbf{w}^{\top}\mathbf{x} + b$, then f is $(\rho_1\|\mathbf{w}\|_2)$ -Lipschitz.

Proof

$$|f(\mathbf{x}_1) - f(\mathbf{x}_2)| \le \rho_1 ||g_2(\mathbf{x}_1) - g_2(\mathbf{x}_2)|| \le \rho_1 \rho_2 ||\mathbf{w}_1 - \mathbf{w}_2||_2$$

Ex14 For binary classification $y \in \{-1,1\}$, $f(\mathbf{w}) = y(\mathbf{w}^{\top}\mathbf{x} + b)$ is $\|\mathbf{x}\|_2$ -Lipschitz following $|f(\mathbf{x}_1) - f(\mathbf{x}_2)| = |y\mathbf{w}_1^{\top}\mathbf{x} - y\mathbf{w}_2^{\top}\mathbf{x}_2| \le \|y\mathbf{x}\|_2 \|\mathbf{w}_1 - \mathbf{w}_2\|_2$. Hence, $\log \log f(\mathbf{w}) = \log(1 + \exp(-y\mathbf{w}^{\top}\mathbf{x}))$ is $\|\mathbf{x}\|_2$ -Lipschitz.

4 Smoothness

Definition 5.8 (smooth function) A differentiable function f is β -smooth if its gradient is β -Lipschitz

remark1. 1

4.4 According to definition, the dual norm of $\|\cdot\|_p (p\geq 1)$ is $\|\theta\|_*=\max_{\mathbf{x}:\|\mathbf{x}\|_p\leq 1}\langle\theta,\mathbf{x}\rangle$. Using the Hölder inequality

$$\|\langle \mathbf{z}, \mathbf{x} \rangle\|_1 \leq \|\mathbf{x}\|_q \|\mathbf{z}\|_p$$

where $\frac{1}{p} + \frac{1}{q} = 1$, we have that:

$$\|\theta\|_* \leq \|\mathbf{x}\|_a \|\mathbf{z}\|_p \leq \|\mathbf{x}\|_a$$

So the dual norm is $\|\cdot\|_q$, where $\frac{1}{p}+\frac{1}{q}=1$.

4.5 Start from strong convexity, we have that

$$\sum_{t=1}^T l_t(\mathbf{x}_t) - \sum_{t=1}^T l_t(\mathbf{u}) \leq \sum_{t=1}^T \left(\frac{1}{2\eta_t} \|\mathbf{x}_t - \mathbf{u}\|_2^2 - \frac{1}{2\eta_t} \|\mathbf{x}_{t+1} - \mathbf{u}\|_2^2 - \frac{\mu_t}{2} \|\mathbf{x}_t - \mathbf{u}\|_2^2 + \frac{\eta_t}{2} \|\mathbf{g}_t\|_2^2 \right)$$

Let all $mu_t \le \mu$, choose $\eta_t = 1/\mu t$. Given that the loss functions are Lipschitz, we can further bound the regret to be

$$\sum_{t=1}^T l_t(\mathbf{x}_t) - \sum_{t=1}^T l_t(\mathbf{u}) \leq \sum_{t=1}^T \frac{\eta_t}{2} \|\mathbf{g}_t\|_2^2 = \frac{L^2}{2\mu} \sum_{t=1}^T \frac{1}{t}$$

Since that the loss functions are smooth, t can be rewrite as $t \geq \sum_{i=1}^t \frac{L \|\mathbf{x} - \mathbf{u}\|_2^2}{\|l_i(\mathbf{x}) - l_i(\mathbf{u})\|_2^2} \geq \frac{L}{M} \sum_{i=1}^t \frac{\|\mathbf{g}_i\|_2^2}{\|l_i(\mathbf{x}) - l_i(\mathbf{u})\|_2^2}$, so $\frac{1}{t} \leq \frac{M}{L} \frac{1}{\sum_{i=1}^t \frac{\|\mathbf{g}_i\|_2^2}{\|l_i(\mathbf{x}) - l_i(\mathbf{u})\|_2^2}}$.

Now using the fact that $\sum_{t=1}^T \frac{1}{t} \leq 1 + \ln T$, we can also make integral by $\|l_i(\mathbf{x}) - l_i(\mathbf{u})\|_2^2$ and get that

$$\sum_{t=1}^T l_t(\mathbf{x}_t) - \sum_{t=1}^T l_t(\mathbf{u}) \leq O(\ln(1 + [\sum_{t=1}^T l_t(\mathbf{x}_t) - \sum_{t=1}^T l_t(\mathbf{u})] \sum_{t=1}^T \sum_{t=1}^T l_t(\mathbf{u})))$$

Using the fact that $x \leq a \ln(1+bx) + c$ leads to $x \leq a \ln(2ab \ln(ab) + 2bc + 2) + c$, it leads to

$$\sum_{t=1}^{T} l_t(\mathbf{x}_t) - \sum_{t=1}^{T} l_t(\mathbf{u}) \le O(1 + \ln \sum_{t=1}^{T} l_t(\mathbf{u})$$

which is the $O(1 + \ln L^*)$ bound.

4.6 With regard to $\|\cdot\|_2$, we need to prove that

$$||l''(\mathbf{x}_1)||_2 \le \frac{1}{4}$$

Note that

$$l'(\mathbf{x}) = \frac{-y\mathbf{z}e^{-y\langle\mathbf{z},\mathbf{x}\rangle}}{1+e^{-y\langle\mathbf{z},\mathbf{x}\rangle}} = -y\mathbf{z}(1-\exp(-l(\mathbf{x})))$$

$$l''(\mathbf{x}) = y\mathbf{z} \exp(-l(\mathbf{x}))(1 - \exp(-l(\mathbf{x})))$$

Since $y \in \{-1, 1\}$ and $\|\mathbf{z}\|_2 \le 1$, we can bound it by

$$||l''(\mathbf{x}_1)||_2 \le |\exp(-l(\mathbf{x}))(1 - \exp(-l(\mathbf{x})))|$$

Note that $l(\mathbf{x}) > 0$, so $0 < \exp(-l(\mathbf{x})) < 1$, so the upper bound is 1/4.