Machine Learning and Neural Networks (MATH3431) Epiphany term, 2024

Handout 1: Elements of convex learning problems

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Aim. To introduce elements of convexity, Lipschitzness, and smoothness that can be used for the analysis of stochastic gradient related learning algorithms.

Reading list & references:

- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
  - Ch. 12 Convex Learning Problems

Further reading

- Bishop, C. M. (2006). Pattern recognition and machine learning. New York: Springer.

1. Motivations

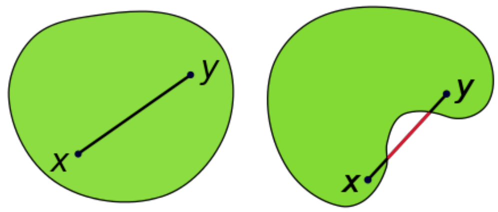
Note 1. We introduce concepts of convexity and smoothness that facilitate the analysis and understanding of the learning problems and their solutions that we will discuss (eg stochastic gradient descent, SVM) later on. Also learning problems with such characteristics can be learned more efficiently.

Note 2. Some of the ML problems discussed in the course (eg, Artificial neural networks, Gaussian process regression) are non-convex. To overcome this problem, we will introduce the concept of surrogate loss function that allows a non-convex problem to be handled with the tools introduced int he convex setting.

2. Convexity

Definition 3. A set C is convex if for any $u, v \in C$ and for any $\alpha \in [0,1]$ we have that $\alpha u + (1-\alpha)\, v \in C$.

Note 4. Namely, a set C is convex if for any $u, v \in C$, the line segment between u and v is contained in C.



(A) (B)

FIGURE 2.1. (2.1a) is a Convex set ; (2.1b) is a non-convex set

Definition 5. Let C be a convex set. A function $f : C \to R$ is convex function if for any $u, v \in C$ and for any $\alpha \in [0, 1]$

$$f(\alpha u + (1 - \alpha) v) \leq \alpha f(u) + (1 - \alpha) f(v)$$

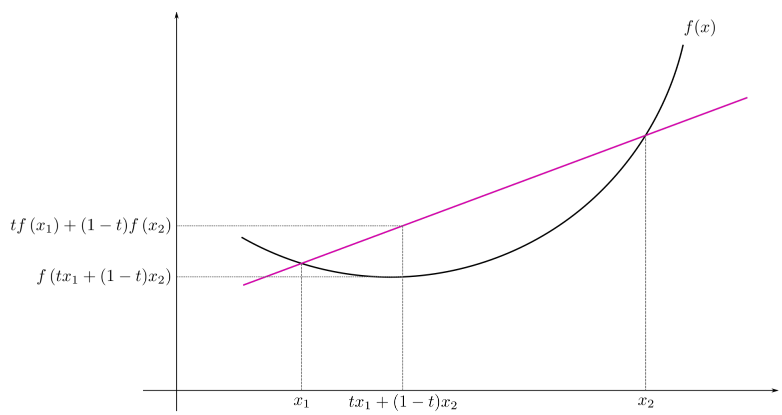


FIGURE 2.2. A convex function

Example 6. The function $f : \mathbb{R} \to \mathbb{R}_+$ with $f(x) = x^2$ is convex function. For any $u, v \in C$ and for any $\alpha \in [0, 1]$ it is

$$(\alpha u + (1 - \alpha) v)^2 - \alpha (u)^2 + (1 - \alpha)(v)^2 = -\alpha (1 - \alpha)(u - v)^2 \leq 0$$

Proposition 7. *Every local minimum of a convex function is the global minimum.*

Proposition 8. *Let $f : C \to \mathbb{R}$ be convex function. The tangent of f at $w \in C$ is below f, namely*

$$\forall u \in C \quad f(u) \geq f(w) + \langle \nabla f(w), u - w \rangle$$

Proposition 9. *Let $f : \mathbb{R}^d \to \mathbb{R}$ such that $f(w) = g(\langle w, x \rangle + y)$ for some $x \in \mathbb{R}^d$, $y \in \mathbb{R}$. If g is convex function then f is convex function.*

Proof. See Exercise 1 in the Exercise sheet. □

Example 10. Consider the regression problem with regressor $x \in \mathbb{R}^d$, and response $y \in \mathbb{R}$ and predictor rule $h(x) = \langle w, x \rangle$. The loss function $\ell(w, (x, y)) = (\langle w, x \rangle - y)^2$ is convex because $g(a) = (a)^2$ is convex and Proposition 9.

Proposition 11. *Let $f_j : \mathbb{R}^d \to \mathbb{R}$ convex functions for $j = 1, ..., r$. Then:*

(1) $g(x) = \max_{\forall j}(f_j(x))$ *is a convex function*
(2) $g(x) = \sum_{j=1}^{r} w_j f_j(x)$ *is a convex function where* $w_j > 0$

Solution.

(1) For any $u, v \in \mathbb{R}^d$ and for any $\alpha \in [0, 1]$

$$\begin{aligned} g(\alpha u + (1-\alpha)v) =& \max_{\forall j}(f_j(\alpha u + (1-\alpha)v)) \\ \leq& \max_{\forall j}(\alpha f_j(u) + (1-\alpha) f_j(v)) && (f_j \text{ is convex}) \\ \leq& \alpha \max_{\forall j}(f_j(u)) + (1-\alpha)\max_{\forall j}(f_j(v)) && (\max(\cdot) \text{ is convex}) \\ \leq& \alpha g(u) + (1-\alpha) g(v) \end{aligned}$$

(2) For any $u, v \in \mathbb{R}^d$ and for any $\alpha \in [0, 1]$

$$\begin{aligned} g(\alpha u + (1-\alpha)v) =& \sum_{j=1}^{r} w_j f_j(\alpha u + (1-\alpha)v) \\ \leq& \alpha \sum_{j=1}^{r} w_j f_j(u) + (1-\alpha)\sum_{j=1}^{r} w_j f_j(v) && (f_j \text{ is convex}) \\ \leq& \alpha g(u) + (1-\alpha) g(v) \end{aligned}$$

Example 12. $g(x) = |x|$ is convex according to Example 11, as $g(x) = |x| = \max(-x, x)$.

3. Strong convexity

Note 13. Strong convexity is a central concept in regularization, e.g. LASSO, as it makes a convex loss function strongly convex by adding a shrinkage term. The re

Definition 14. (Strongly convex functions) A function f is λ-strongly convex function is for all w, u, and $\alpha \in (0, 1)$ we have

$$f(aw + (1-\alpha)u) \leq af(w) + (1-\alpha) f(u) - \frac{\lambda}{2}\alpha(1-\alpha)\|w-u\|^2 \tag{3.1}$$

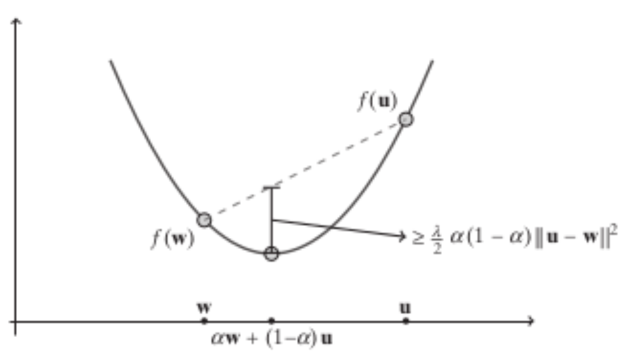


Figure 3.1. Strongly convex function

Proposition 15.

(1) *The function* $f(w) = \lambda \|w\|^2$ *is* 2λ-strongly convex

(2) *If* f *is* λ-strongly convex and g is convex then $f+g$ is λ-strongly convex

Example 16. If $f$is λ-strongly convex and u is a minimizer of f then for any w

$$f(w) - f(u) \geq \frac{\lambda}{2} \|w-u\|^2$$

Hint:: Use the definition, and set $\alpha \to 0$.

Solution. From the definition I have

$$f(aw + (1-\alpha)u) \leq af(w) + (1-\alpha) f(u) - \frac{\lambda}{2}\alpha(1-\alpha)\|w-u\|^2 \Leftrightarrow$$

$$\frac{f(aw+(1-\alpha)u) - f(u)}{\alpha} \leq f(w) - f(u) - \frac{\lambda}{2}\alpha(1-\alpha)\|w-u\|^2 \overset{\alpha \to 0}{\Leftrightarrow}$$

$$\left.\frac{\mathrm{d}}{\mathrm{d}\alpha} g(\alpha)\right|_{\alpha=0} \leq f(w) - f(u) - \frac{\lambda}{2}\|w-u\|^2$$

u is the minimizer of f, then 0 is the minimizer of $g(\alpha) = f(aw + (1-\alpha)u)$, hence $g'(0) = 0$.

4. Lipschitzness

Definition 17. Let $C \in \mathbb{R}^d$. Function $f : \mathbb{R}^d \to \mathbb{R}^k$ is ρ-Lipschitz over C if for every $w_1, w_2 \in C$ we have that

$$\|f(w_1) - f(w_2)\| \leq \rho \|w_1 - w_2\|. \qquad \text{Lipschitz condition} \tag{4.1}$$

Conclusion 18. That means: a Lipschitz function $f(x)$ cannot change too drastically wrt x.

Example 19. Consider the function $f : \mathbb{R} \to \mathbb{R}_+$ with $f(x) = x^2$.

(1) f is not a ρ-Lipschitz in $\mathbb{R}$.

(2) f is a ρ-Lipschitz in $C = \{x \in \mathbb{R} : |x| < \rho/2\}$.

$$|f(x_2) - f(x_1)| = \left|x_2^2 - x_1^2\right| = |(x_2+x_1)(x_2-x_1)| \leq 2\rho/2\,(x_2 - x_1) = \rho|x_2 - x_1|$$

Solution.

(1) For $x_1 = 0$ and $x_2 = 1+\rho$, it is

$$|f(x_2) - f(x_1)| = (1+\rho)^2 > \rho(1+\rho) = \rho|x_2 - x_1|$$

(2) It is

$$|f(x_2) - f(x_1)| = \left|x_2^2 - x_1^2\right| = |(x_2+x_1)(x_2-x_1)| \leq 2\rho/2\,(x_2 - x_1) = \rho|x_2 - x_1|$$

Theorem 20. *Let functions* g_1 *be* ρ_1*-Lipschitz and* g_2 *be* ρ_2*-Lipschitz. Then* f *with* $f(x) = g_1(g_2(x))$ *is* $\rho_1\rho_2$*-Lipschitz.*

Solution. See Exercise 2 from the exercise sheet

Example 21. Let functions g be ρ-Lipschitz. Then f with $f(x) = g(< v, x > +b)$ is $(\rho|v|)$-Lipschitz.

Solution. It is

$$\left|f\left(w_1\right)-f\left(w_2\right)\right| = \left|g\left(< v, w_1 > +b\right)-g\left(< v, w_2 > +b\right)\right| \leq \rho\left|< v, w_1 > +b- < v, w_2 > -b\right|$$
$$\leq \rho\left|v^{\top} w_1-v^{\top} w_2\right| \leq \rho|v|\left|w_1-w_2\right|$$

Note 22. So, given Examples 19 and 21, in the linear regression setting using loss $\ell(w, z=(x, y))= \left(w^{\top} x-y\right)^2$, the loss function is -Lipschitz for a given $z=(x, y)$ and and bounded $\|w\|<\rho$.

5. Smoothness

Definition 23. A differentiable function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is β-smooth if its gradient is β-Lipschitz; namely for all $v, w \in \mathbb{R}^d$

$$\left\|\nabla f\left(w_1\right)-\nabla f\left(w_2\right)\right\| \leq \beta\left\|w_1-w_2\right\| . \tag{5.1}$$

Theorem 24. *Function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is β-smooth iff*

$$f(v) \leq f(w)+<\nabla f(w), v-w>+\frac{\beta}{2}\|v-w\|^2 \tag{5.2}$$

Remark 25. If $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is β-smooth then (5.2) holds, and if it is convex as well then

$$f(v) \geq f(w)+\langle\nabla f(w), v-w\rangle$$

holds. Hence together these conditions imply upper and lower bounds

$$f(v)-f(w) \in\left(\langle\nabla f(w), v-w\rangle,\langle\nabla f(w), v-w\rangle+\frac{\beta}{2}\|v-w\|^2\right)$$

Example 26. If $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is β-smooth then for $v, w \in \mathbb{R}^d$ such that $v=w-\frac{1}{\beta} \nabla f(w)$ then by (5.2), it is

$$\frac{1}{2 \beta}\|\nabla f(w)\|^2 \leq f(w)-f(v)$$

If additionally $f(x)>0$ for all $x \in \mathbb{R}^d$ then

$$\|\nabla f(w)\|^2 \leq 2 \beta f(w)$$

which provides assumptions to bound the gradient.

Theorem 27. *Let $f: \mathbb{R}^d \rightarrow \mathbb{R}$ with $f(w)=g(\langle w, x\rangle+y)$ $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Let $g: \mathbb{R} \rightarrow \mathbb{R}$ be a β-smooth function. Then f is a $\left(\beta\|x\|^2\right)$-smooth.*

Proof. See Exercise 3 from the Exercise sheet □

Example 28. Let $f(w)=(< w, x > +y)^2$ for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Then f is $\left(2\|x\|^2\right)$-smooth.

Solution. It is $f(w)=g(< w, x > +y)$ for $g(a)=a^2$. g is 2-smooth since

$$\left\|g^{\prime}\left(w_1\right)-g^{\prime}\left(w_2\right)\right\|=\left\|2 w_1-2 w_2\right\| \leq 2\left\|w_1-w_2\right\| .$$

Hence from (27), f is $\left(2\|x\|^2\right)$-smooth.

Example 29. Consider the regression problem with predictor rule $h(x) = \langle w, x\rangle$, loss function $\ell(w,(x,y)) = (\langle w, x\rangle - y)^2$, feature $x \in \mathbb{R}^d$, and target $y \in \mathbb{R}$. Then $\ell(w,\cdot)$ is $\left(2\|x\|^2\right)$-smooth.

Solution. Follows from Example 28.

6. Convex learning problems

Definition 30. Convex learning problem is a learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ that the hypothesis class $\mathcal{H}$ is a convex set, and the loss function ℓ is a convex function for each example $z \in \mathcal{Z}$.

Example 31. Consider the regression problem with predictor rule $h(x) = \langle w, x\rangle$, loss function $\ell(w,(x,y)) = (\langle w, x\rangle - y)^2$, feature $x \in \mathbb{R}^d$, and target $y \in \mathbb{R}$. This imposes a convex learning problem due to Example 11.

Definition 32. Convex-Lipschitz-Bounded Learning Problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with parameters ρ, and B, is called the learning problem whose the hypothesis class $\mathcal{H}$ is a convex set, for all $w \in \mathcal{H}$ it is $\|w\| \le B$, and the loss function $\ell(\cdot, z)$ is convex and ρ-Lipschitz function for all $z \in \mathcal{Z}$.

Example 33. Consider the regression problem with predictor rule $h(x) = \langle w, x\rangle$, loss function $\ell(w,(x,y)) = (\langle w, x\rangle - y)^2$, feature $x \in \mathbb{R}^d$, and target $y \in \mathbb{R}$. This imposes a Convex-Lipschitz-Bounded Learning Problem if $\mathcal{H} = \left\{w \in \mathbb{R}^d : \|w\| \le B\right\}$ due to Examples 11, and 19(2).

Definition 34. Convex-Smooth-Bounded Learning Problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with parameters β, and B, is called the learning problem whose the hypothesis class $\mathcal{H}$ is a convex set, for all $w \in \mathcal{H}$ it is $\|w\| \le B$, and the loss function $\ell(\cdot, z)$ is convex, nonnegative, and β-smooth function for all $z \in \mathcal{Z}$.

Example 35. Consider the regression problem with predictor rule $h(x) = \langle w, x\rangle$, loss function $\ell(w,(x,y)) = (\langle w, x\rangle - y)^2$, feature $x \in \mathbb{R}^d$, and target $y \in \mathbb{R}$. This imposes a Convex-Smooth-Bounded Learning Problem if $\mathcal{H} = \left\{w \in \mathbb{R}^d : \|w\| \le B\right\}$ due to Examples 11, and 29.

7. Non-convex learning problems (surrogate treatment)

Remark 36. A learning problem may involve non-convex loss function $\ell(w,z)$ which implies a non-convex risk function $R_g(w)$. However, our learning algorithm will be analyzed in the convex setting. A suitable treatment to overcome this difficulty would be to upper bound the non-convex loss function $\ell(w,z)$ by a convex surrogate loss function $\tilde{\ell}(w,z)$ for all w, and use $\tilde{\ell}(w,z)$ instead of $\ell(w,z)$.

Example 37. Consider the binary classification problem with inputs $x \in \mathcal{X}$, outputs $y \in \{-1,+1\}$; we need to learn $w \in \mathcal{H}$ from hypothesis class $\mathcal{H} \subset \mathbb{R}^d$ with respect to the loss

$$\ell(w,(x,y)) = 1_{(y\langle w,x\rangle \le 0)}$$

with $y \in \mathbb{R}$, and $x \in \mathbb{R}^d$. Here $\ell(\cdot)$ is non-convex. A convex surrogate loss function can be

$$\tilde{\ell}(w,(x,y)) = \max(0, 1 - y\langle w, x\rangle)$$

which is convex (Example 11) wrt w. Note that:

- $\tilde{\ell}\left(w,(x,y)\right)$ is convex wrt w ; because $\max\left(\cdot\right)$ is convex
- $\ell\left(w,(x,y)\right)\le\tilde{\ell}\left(w,(x,y)\right)$ for all $w\in\mathcal{H}$

Then we can compute

$$\tilde{w}_{*}=\arg\min_{\forall x}\left(\tilde{R}_{g}\left(w\right)\right)=\arg\min_{\forall x}\left(\mathrm{E}_{(x,y)\sim g}\left(\max\left(0,1-y\langle w,x\rangle\right)\right)\right)$$

instead of

$$w_{*}=\arg\min_{\forall x}\left(R_{g}\left(w\right)\right)=\arg\min_{\forall x}\left(\mathrm{E}_{(x,y)\sim g}\left(1_{(y\langle w,x\rangle\le0)}\right)\right)$$

Of course by using the surrogate loss instead of the actuall one, we introduce some approximation error in the produced output $\tilde{w}_{*}\neq w_{*}$.

Remark 38. (Intuitions...) Using a convex surrogate loss function instead the convex one, facilitates computations but introduces extra error to the solution. If $R_{g}(\cdot)$ is the risk under the non-convex loss, $\tilde{R}_{g}(\cdot)$ is the risk under the convex surrogate loss, and $\tilde{w}_{\mathrm{alg}}$ is the output of the learning algorithm under $\tilde{R}_{g}(\cdot)$ then we have the upper bound

$$R_{g}(\tilde{w}_{\mathrm{alg}})\le\underbrace{\min_{w\in\mathcal{H}}\left(R_{g}(w)\right)}_{\mathrm{I}}+\underbrace{\left(\min_{w\in\mathcal{H}}\left(\tilde{R}_{g}(w)\right)-\min_{w\in\mathcal{H}}\left(R_{g}(w)\right)\right)}_{\mathrm{II}}+\underbrace{\epsilon}_{\mathrm{III}}$$

where term I is the approximation error measuring how well the hypothesis class performs on the generating model, term II is the optimization error due to the use of surrogate loss instead of the actual non-convex one, and term III is the estimation error due to the use of a training set and not the whole generation model.