Machine Learning and Neural Networks (MATH3431) Epiphany term, 2023

Handout 1: Elements of convex learning problems

Lecturer & author: Georgios P. Karagiannis georgios.karagiannis@durham.ac.uk

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:

- Bishop, C. M. (2006). Pattern recognition and machine learning. New York: Springer.
- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.

1. Motivations

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

Note 2. Most of the ML problems discussed in the course (eg, Artificial neural networks, Gaussian process regression) are usually non-convex.

Note 3. 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. Convex learning problems

Definition 4. 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 5. Multiple linear regression $< w, x > \to y$ with $y \in \mathbb{R}$, hypothesis class $\mathcal{H} = \left\{w \in \mathbb{R}^d\right\}$ and loss $\ell\left(w, (x, y)\right) = \left(< w, x > -y\right)^2$ with

$$w^* = \arg\min_{\forall w} \mathrm{E}\left(< w, x > -y\right)^2$$

or

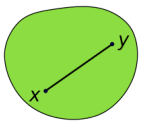
$$w^{**} = \arg\min_{\forall w} \frac{1}{m} \sum_{i=1}^{m} \left(< w, x_i > -y\right)^2$$

is a convex learning problem for reasons that will be discussed below.

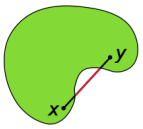
3. Convexity

Definition 6. A set C is convex if for any $u, v \in C$, the line segment between u and v is contained in C. Namely,

- for any $u, v \in C$ and for any $\alpha \in [0, 1]$ we have that $\alpha u + (1 - \alpha) v \in C$.



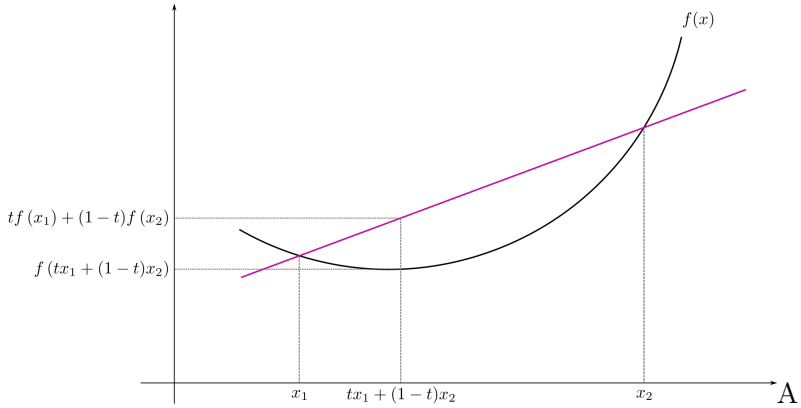
A convex set



A non-convex set

Definition 7. 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 $\alpha \in [0, 1]$

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



A convex function

Example 8. 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 9. *Every local minimum of a convex function is the global minimum.*

Proposition 10. *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 11. *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 12. Consider the regression problem $x \mapsto y$ with $x \in \mathbb{R}^d$, $y \in \mathbb{R}$ and predictor $h(x) = \langle w, x \rangle$. The loss function $\ell(w, (x, y)) = (\langle w, x \rangle + y)^2$ is convex because $g(a) = (a)^2$ is convex and Proposition 11.

Example 13. 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 14. $g(x) = |x|$ is convex according to Example 13, as $g(x) = |x| = \max(-x, x)$.

4. Lipschitzbness

Definition 15. 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 16. That means: a Lipschitz function $f(x)$ cannot change too drastically wrt x.

Example 17. 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 18. *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 19. Let functions g be ρ-Lipschitz. Then f with $f(x) = g(< v, x > +b)$ is $(\rho|v|)$-Lipschitz.

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

Note 20. So, given Examples 17 and 19, in the linear regression setting using loss $\ell(w, z) = \left(w^\top x - z\right)^2$, the loss unction is -Lipschitz for a given z and and bounded $\|w\| < \rho$.

5. Smoothness

Definition 21. A differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is β-smooth if its gradient is β-Lipschitz; namely for all $v, w \in \mathbb{R}^d$

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

Theorem 22. *Function $f : \mathbb{R}^d \to \mathbb{R}$ is β-smooth iff*

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

Remark 23. If $f : \mathbb{R}^d \to \mathbb{R}$ is β-smooth then (5.2) holds, and if it is convex as well then

$$f(v) \geq f(w) + < \nabla f(w), v - w >$$

holds. Hence if both conditions imply upper and lower bounds

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

Remark 24. If $f : \mathbb{R}^d \to \mathbb{R}$ 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 25. *Let $f : \mathbb{R}^d \to \mathbb{R}$ with $f(w) = g(\langle w, x \rangle + y)$ $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Let $g : \mathbb{R} \to \mathbb{R}$ be a β-smooth function. Then f is a $\left(\beta \|x\|^2\right)$-smooth.*

Solution. See Exercise 3 from the Exercise sheet

Example 26. 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

$$\left\|g'(w_1) - g'(w_2)\right\| = \|2w_1 - 2w_2\| \leq 2 \|w_1 - w_2\|.$$

Hence from (25), f is $\left(2 \|x\|^2\right)$-smooth.

Remark 27. A 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 28. 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

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

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 14) wrt w. Note that:

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

Then we can compute

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

instead of

$$w_* = \arg\min_{\forall x}\left(R_g(w)\right) = \arg\min_{\forall x}\left(\mathrm{E}_{(x,y)\sim g}\left(1_{(y\langle w,x\rangle \leq 0)}\right)\right)$$

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 29. (Intuitions...) Using a convex surrogate loss function instead the convex one, fascilitates 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 $\tilde{w}_{\text{alg}}$ is the output of the learning algorithm under $\tilde{R}_g(\cdot)$ then we have the upper bound

$$R_g(\tilde{w}_{\text{alg}}) \leq \underbrace{\min_{w\in\mathcal{H}}\left(R_g(w)\right)}_{\text{I}} + \underbrace{\left(\min_{w\in\mathcal{H}}\left(\tilde{R}_g(w)\right) - \min_{w\in\mathcal{H}}\left(R_g(w)\right)\right)}_{\text{II}} + \underbrace{\epsilon}_{\text{III}}$$

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.