Machine Learning and Neural Networks (MATH3431)

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Lecture notes 2: Elements of convex learning problems

Lecturer & author: Georgios P. Karagiannis

georgios.karagiannis@durham.ac.uk

Aim. To introduce convex learning problems that can be used as a framework 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 learning problems associated with convexity, Lipschitzness and smoothness to be able to analyze and understand the machine learning (ML) tools we will discuss later on (eg stochastic gradient descent, SVM). We discuss ways allowing to address nonconvex ML problems (eg, Artificial neural networks, Gaussian process regression) in the convex setting.

2. Convexity

Note 2. Convexity is a central concept in learning, e.g. least squares, as it often considers a Euclidean distance as a Risk function to be minimized.

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

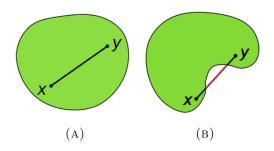


FIGURE 2.1. (2.1a) is a Convex set; (2.1b) is a non-convex set

Example 4. For instance \mathbb{R}^d for $d \geq 1$ is a 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 $\alpha \in [0, 1]$

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

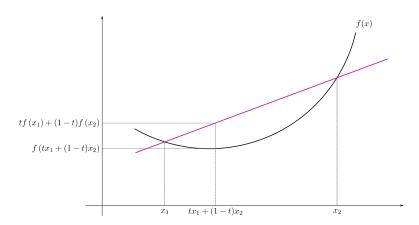


Figure 2.2. A convex function

Example 6. The function $f: \mathbb{R}^d \to \mathbb{R}_+$ with $f(x) = ||x||_2^2$ is convex function. For any $u, v \in C$ and for any $\alpha \in [0, 1]$ it is

$$\begin{aligned} &\|\alpha u + (1 - \alpha) v\|_{2}^{2} - \alpha \|u\|_{2}^{2} - (1 - \alpha) \|v\|_{2}^{2} \\ &= (\alpha u + (1 - \alpha) v)^{\top} (\alpha u + (1 - \alpha) v) - \alpha \|u\|_{2}^{2} - (1 - \alpha) \|v\|_{2}^{2} \\ &= \dots = -\alpha (1 - \alpha) \|u - v\|_{2}^{2} \le 0 \end{aligned}$$

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

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

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

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.

Note 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 $w_j > 0$

Proof.

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

$$g(\alpha u + (1 - \alpha) v) = \max_{\forall j} (f_j(\alpha u + (1 - \alpha) v))$$

$$\leq \max_{\forall j} (\alpha f_j(u) + (1 - \alpha) f_j(v)) \qquad (f_j \text{ is convex})$$

$$\leq \alpha \max_{\forall j} (f_j(u)) + (1 - \alpha) \max_{\forall j} (f_j(v)) \qquad (\max(\cdot) \text{ is convex})$$

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

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

$$g(\alpha u + (1 - \alpha) v) = \sum_{j=1}^{r} w_j f_j (\alpha u + (1 - \alpha) v)$$

$$\leq \alpha \sum_{j=1}^{r} w_j f_j (u) + (1 - \alpha) \sum_{j=1}^{r} w_j f_j (v) \qquad (f_j \text{ is convex})$$

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

Example 12. $g(x) = ||x||_1$ is convex according to Note 11, since $|x_j| = \max(-x_j, x_j)$ and $||x||_1 = \sum_j |x_j|$.

3. Strong convexity

Note 13. Strong convexity is a central concept in Ridge regularization, as it makes a convex loss function strongly convex by adding a shrinkage term.

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

(3.1)
$$f(\alpha w + (1 - \alpha) u) \le \alpha f(w) + (1 - \alpha) f(u) - \frac{\lambda}{2} \alpha (1 - \alpha) \|w - u\|^2$$

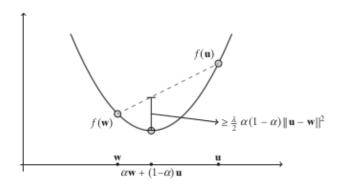


FIGURE 3.1. Strongly convex function

Note 15. The following can be checked from the definition by substitution

- (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

4. Lipschitzness

Definition 16. Let $C \subseteq \mathbb{R}^d$. Function $f: C \to \mathbb{R}^k$ is ρ -Lipschitz over C if for every $w_1, w_2 \in C$ we have that

(4.1)
$$||f(w_1) - f(w_2)|| \le \rho ||w_1 - w_2||$$
. Lipschitz condition

Note 17. That means: a Lipschitz function f(x) cannot change too drastically wrt x.

Example 18. 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 $C = \{x \in \mathbb{R} : |x| < \rho/2\}$.

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

$$|f(x_2) - f(x_1)| = |x_2^2 - x_1^2| = |(x_2 + x_1)(x_2 - x_1)| \le 2\rho/2(x_2 - x_1) = \rho |x_2 - x_1|$$

Note 19. 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.

[See Exercise 2 from the exercise sheet]

Example 20. Let functions g be ρ -Lipschitz. Then f with $f(x) = g(\langle v, x \rangle + b)$ is $(\rho |v|)$ -Lipschitz.

Solution. It is

$$|f(w_1) - f(w_2)| = |g(\langle v, w_1 \rangle + b) - g(\langle v, w_2 \rangle + b)| \le \rho |\langle v, w_1 \rangle + b - \langle v, w_2 \rangle - b|$$

$$\le \rho |v^\top w_1 - v^\top w_2| \le \rho |v| |w_1 - w_2|$$

Note 21. So, given Examples 18 and 20, in the linear regression setting using loss $\ell(w, z = (x, y)) = (w^{\top}x - y)^2$, the loss function is -Lipschitz for a given z = (x, y) and and bounded $||w|| < \rho$.

5. Smoothness

Definition 22. A differentiable function $f: \mathbb{R}^d \to \mathbb{R}$ is β -smooth if its gradient is β -Lipschitz; namely for all $v, w \in \mathbb{R}^d$

$$\|\nabla f(w_1) - \nabla f(w_2)\| \le \beta \|w_1 - w_2\|.$$

Note 23. Function $f: \mathbb{R}^d \to \mathbb{R}$ is β -smooth iff

(5.2)
$$f(v) \le f(w) + \langle \nabla f(w), v - w \rangle + \frac{\beta}{2} \|v - w\|^2$$

Note 24. 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 $(\beta ||x||^2)$ -smooth.

[See Exercise 3 from the Exercise sheet]

Example 25. Let $f(w) = (\langle w, x \rangle + y)^2$ for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Then f is $(2 ||x||^2)$ -smooth. To show that we set $f(w) = g(\langle w, x \rangle + y)$ where $g(a) = a^2$. g is 2-smooth since

$$\|g'(w_1) - g'(w_2)\| = \|2w_1 - 2w_2\| \le 2 \|w_1 - w_2\|.$$

Hence from Theorem 24, f is $(2||x||^2)$ -smooth.

Example 26. 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 $(2 ||x||^2)$ -smooth.

[Follows from Example 25.]

6. Convex Learning Problems

Definition 27. 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 $\ell(\cdot, z)$ is a convex function for each example $z \in \mathcal{Z}$.

Example 28. 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 Examples 4 and 11.

Definition 29. 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 $||w|| \leq B$, and the loss function $\ell(\cdot, z)$ is convex and ρ -Lipschitz function for all $z \in \mathcal{Z}$.

Example 30. 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 $\mathcal{H} = \{w \in \mathbb{R}^d : ||w|| \leq B\}$ due to Examples 11, and 18(2).

Definition 31. 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 $||w|| \leq B$, and the loss function $\ell(\cdot, z)$ is convex, nonnegative, and β -smooth function for all $z \in \mathcal{Z}$.

Example 32. 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 $\mathcal{H} = \{w \in \mathbb{R}^d : ||w|| \leq B\}$ due to Examples 11, and 26.

Note 33. (Empirical risk minimization learning problem) If ℓ is a convex loss function and the class \mathcal{H} is convex, then the ERM_{\mathcal{H}} problem, of minimizing the empirical risk $\hat{R}_{\mathcal{S}}(w)$ over \mathcal{H} , is a convex optimization problem

Proof. The Empirical risk minimization (ERM) problem $(\mathcal{H}, \mathcal{Z}, \ell)$ is

$$w^* = \operatorname*{arg\,min}_{w \in \mathcal{H}} \left\{ \hat{R}_{\mathcal{S}} \left(w \right) \right\}$$

given a sample $S = \{z_1, ..., z_m\}$ for $\hat{R}_S(w) = \frac{1}{m} \sum_{i=1}^m \ell(w, z_i)$. $\hat{R}_S(w)$ is a convex function from Note (11). Hence ERM rule is a problem of minimizing a convex function subject to the constraint that the solution should be in a convex set.

Example 34. Multiple linear regression 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 $y \in \mathbb{R}$ where

$$w^* = \underset{w}{\operatorname{arg\,minE}} \left(\langle w, x \rangle - y \right)^2$$

or

$$w^{**} = \underset{w}{\operatorname{arg\,min}} \frac{1}{m} \sum_{i=1}^{m} \left(\langle w, x_i \rangle - y_i \right)^2$$

is a convex learning problem –from Note 33.

Note 35. (Ridge / ℓ_2 -RLM problem) If ℓ is a convex loss function w.r.t. w, the class \mathcal{H} is convex, and $J(\cdot; \lambda) = \lambda \|\cdot\|_2^2$ with $\lambda > 0$ then $\hat{R}_{\mathcal{S}}(w) + \lambda \|w\|_2^2$ is a 2λ -strongly convex function, and hence the ℓ_2 -RLM problem

$$w^* = \operatorname*{arg\,min}_{w \in \mathcal{H}} \left\{ \hat{R}_{\mathcal{S}}\left(w\right) + \lambda \left\|w\right\|_2^2 \right\}$$

is a strongly convex optimization problem (i.e. the learning rule is the minimizer of a strongly convex function over a convex set).

Proof. $\hat{R}_{\mathcal{S}}(\cdot)$ is a convex function from Note 33, $\lambda \|\cdot\|_2^2$ is 2λ -strongly convex, hence $\hat{R}_{\mathcal{S}}(w) + \lambda \|w\|_2^2$ is a 2λ -strongly convex function. Hence the above Ridge RLM problem is a strongly convex optimization problem.

7. Non-convex learning problems (surrogate treatment)

Note 36. A learning problem may involve non-convex loss function $\ell(w, z)$ w.r.t. w which implies a non-convex risk function $R_g(w)$. A suitable treatment to analyze the associated learning tools within the convex setting 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

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

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:

- $\tilde{\ell}(w,(x,y))$ 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

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

instead of

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

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

Note 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}_{alg} is the output of the learning algorithm under $\tilde{R}_g(\cdot)$ then we have the upper bound

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

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.