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

Handout 2: 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

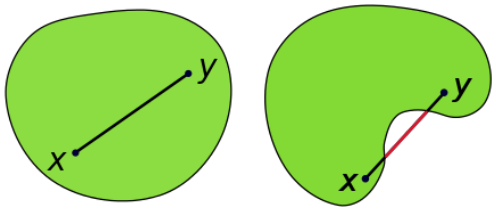
Note 1. We introduce concepts of convexity and smoothness that facilitate the analysis and understanding of the learning problems and their solutions that we will discuss (eg stochastic gradient descent, SVM) later on. Also learning problems with such characteristics can be learned more efficiently.

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

Example 5. For instance $\mathbb{R}^d$ for $d \geq 1$ is a convex set.

Definition 6. 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 $\alpha \in [0, 1]$

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

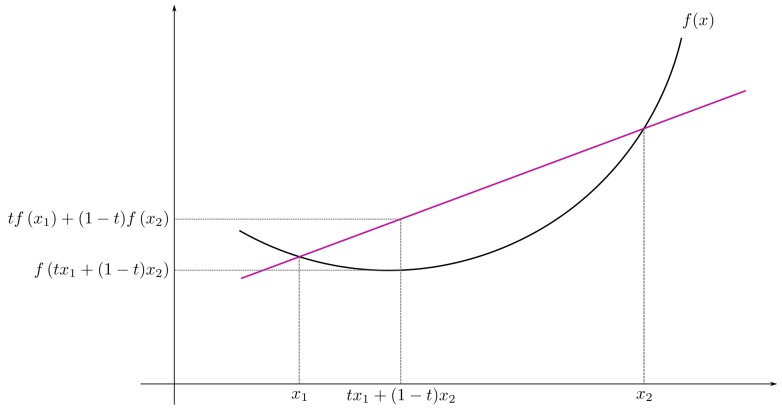


FIGURE 2.2. A convex function

Example 7. 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

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

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

Proposition 9. *Let $f : C \to \mathbb{R}$ be convex function. The tangent of f at $w \in C$ is below f, namely*

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

Proposition 10. *Let $f : \mathbb{R}^d \to \mathbb{R}$ such that $f\left(w\right) = g\left(\left\langle w, x\right\rangle + y\right)$ 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 11. 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 10.

Proposition 12. *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 13. $g(x) = |x|$ is convex according to Example 12, as $g(x) = |x| = \max(-x, x)$.

3. Lipschitzness

Definition 14. 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

$$\|f(w_1) - f(w_2)\| \leq \rho \|w_1 - w_2\|. \qquad \text{Lipschitz condition} \tag{3.1}$$

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

Example 16. 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 17. *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 18. Let functions g be ρ-Lipschitz. Then f with $f(x) = g(< v, x > +b)$ is $(\rho\,|v|)$-Lipschitz.

Solution. It is

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

Note 19. So, given Examples 16 and 18, 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 $\|w\| < \rho$.

4. Smoothness

Definition 20. A differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is β-smooth if its gradient is β-Lipschitz; namely for all $v, w \in \mathbb{R}^d$

$$\|\nabla f(w_1) - \nabla f(w_2)\| \leq \beta\,\|w_1 - w_2\|\,. \tag{4.1}$$

Theorem 21. *Function $f : \mathbb{R}^d \to \mathbb{R}$ is β-smooth iff*

$$f(v) \leq f(w) + \langle \nabla f(w), v - w\rangle + \frac{\beta}{2}\,\|v - w\|^2 \tag{4.2}$$

Theorem 22. *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.*

Proof. See Exercise 3 from the Exercise sheet □

Example 23. 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 Theorem 22, f is $\left(2\,\|x\|^2\right)$-smooth.

Example 24. 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 23.

5. Convex learning problems

Definition 25. 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 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 $y \in \mathbb{R}$. This imposes a convex learning problem due to Examples 5 and 12.

Definition 27. 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 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-Lipschitz-Bounded Learning Problem if $\mathcal{H} = \left\{w \in \mathbb{R}^d : \|w\| \leq B\right\}$ due to Examples 12, and 16(2).

Definition 29. 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 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-Smooth-Bounded Learning Problem if $\mathcal{H} = \left\{w \in \mathbb{R}^d : \|w\| \leq B\right\}$ due to Examples 12, and 24.

Proposition 31. *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 (that is, a problem of minimizing a convex function over a convex set).*

Proof. The ERM$_\mathcal{H}$ problem is

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

given a sample $\mathcal{S} = \{z_1, ..., z_m\}$ for $\hat{R}_\mathcal{S}(w) = \frac{1}{m}\sum_{i=1}^m \ell(w, z_i)$. $\hat{R}_\mathcal{S}(w)$ is a convex function from Proposition (12). 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 32. 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

$$w^* = \arg\min_w \mathrm{E}\,(\langle w, x\rangle - y)^2$$

or

$$w^{**} = \arg\min_w \frac{1}{m}\sum_{i=1}^m (\langle w, x_i\rangle - y_i)^2$$

is a convex learning problem –from Proposition 31.

Note 33. Problems like that in Proposition 31 can be efficiently solved with algorithms such as Stochastic Gradients Descent to be introduced later.

6. Non-convex learning problems (surrogate treatment)

Remark 34. 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 35. 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 12) 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 actual one, we introduce some approximation error in the produced output $\tilde{w}_* \neq w_*$.

Remark 36. (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 $\tilde{w}_{\text{alg}}$ 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.

7. Strong convexity

Note 37. Strong convexity is a central concept in regularization, e.g. Ridge, as it makes a convex loss function strongly convex by adding a shrinkage term.

Definition 38. (Strongly convex functions) A function f is λ-strongly convex function is for all w, u, and $\alpha \in (0,1)$ we have

$$f(aw + (1-\alpha)u) \leq af(w) + (1-\alpha)f(u) - \frac{\lambda}{2}\alpha(1-\alpha)\|w-u\|^2 \tag{7.1}$$

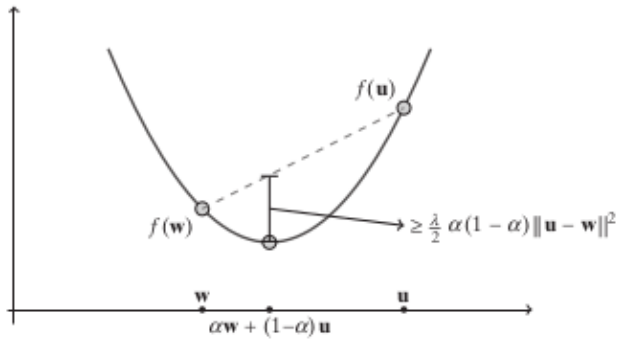


FIGURE 7.1. Strongly convex function

Proposition 39.

(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

Proof. Both can be checked from the definition by substitution. □

Lemma 40. *If* f *is* λ-strongly convex and $w^* = \arg\min_w f(w)$ is a minimizer of f then for any w

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

Proof. Exercise 7 in the Exercise sheet. □

Proposition 41. *If* ℓ *is a convex loss function and the class* $\mathcal{H}$ *is convex, then the Ridge ERM*$_\mathcal{H}$ *problem, with learning rule*

$$\mathfrak{A}(\mathcal{S}) = \arg\min_{w\in\mathcal{H}} \left(\hat{R}_\mathcal{S}(w) + \lambda\|w\|_2^2\right)$$

is a 2λ-strongly convex learning problem.

Proposition 42. *(*ERM *with Ridge regularization) If* ℓ *is a convex loss function, 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 the ERM*$_\mathcal{H}$ *problem*

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

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 Proposition 31, $\lambda\|\cdot\|_2^2$ is 2λ-strongly convex, hence $\hat{R}_\mathcal{S}(w) + \lambda\|w\|_2^2$ is a 2λ-strongly convex function. Hence the above ERM$_\mathcal{H}$ problem is a strongly convex optimization problem. □