Machine Learning Theory: Introduction

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1 Something different: Gradient descend convergence for β -smooth function

You need three definitions and theorems for β -smooth function:

1. **definition** of convex function:

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle$$
 (1)

2. **definition** of β -smooth convex function requires:

$$\|\nabla f(x) - \nabla f(y)\| \le \beta \|x - y\|^2 \tag{2}$$

QUESTION: what kind of function is $\nabla f(\cdot)$?

3. **Theorem 1** if convex function f is β -smooth, then for gradient descend $x_{t+1} = x_t - \eta \nabla f(x_t)$ and when $\eta = \frac{1}{\beta}$, we have:

$$f(x_{t+1}) \le f(x_t) - \frac{\eta}{2} \|\nabla f(x_t)\|_2^2$$
 (3)

QUESTION: what does it tell you about β -smooth convex function guarantees?

Theorem 2 if convex function f is β -smooth, for gradient descend $x_{t+1} = x_t - \eta \nabla f(x)$, with learning rate $\eta = \frac{1}{\beta}$, then:

$$\implies \epsilon \equiv f(x_T) - f(x^*) \le \frac{1}{T} \sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*)$$

$$\le \frac{1}{T} \frac{1}{2\eta} \left(\|x_0 - x^*\|_2^2 - \|x_T - x^*\|_2^2 \right)$$
(4)

- 1. which means $\epsilon(t)=O(\frac{1}{t})$, in word, it says it takes $t\times$ "some constant" iterations to achieve error $\frac{1}{\epsilon}$
- 2. first inequality line is due to Theorem 1

The **proof** began by Eq.(3), conditioned on $\eta = \frac{1}{\beta}$:

$$f(x_{t+1}) \le f(x_t) - \frac{\eta}{2} \|\nabla f(x_t)\|_2^2$$

$$\le f(x^*) + \langle \nabla f(x_t), x_t - x^* \rangle - \frac{\eta}{2} \|\nabla f(x_t)\|_2^2 \qquad \text{we need to bring in } x^*$$
(5)

QUESTION: how do you get the red part?

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle$$

$$f(x^*) \ge f(x_t) + \langle \nabla f(x_t), x^* - x_t \rangle$$

$$\implies -f(x^*) \le -f(x_t) + \langle \nabla f(x_t), x_t - x^* \rangle$$

$$\implies f(x_t) \le f(x^*) + \langle \nabla f(x_t), x_t - x^* \rangle$$
(6)

looking at Eq.(5), we need to expand $\langle \nabla f(x_t), x_t - x^* \rangle$. The **first attempt** is:

$$||a - b||_{2}^{2} = ||a||_{2}^{2} - 2\langle a, b \rangle + ||b||_{2}^{2}$$

$$\implies \langle a, b \rangle = \frac{||a||_{2}^{2} + ||b||_{2}^{2} - ||a - b||_{2}^{2}}{2}$$
(7)

so by letting $a = x_t - x^*$, and $b = \nabla f(x_t)$, we have:

$$f(x_{t+1}) \le f(x^*) + \frac{1}{2} \left(\|x_t - x^*\|_2^2 + \|\nabla f(x_t)\|_2^2 - \|x_t - x^* - \nabla f(x_t)\|_2^2 - \eta \|\nabla f(x_t)\|_2^2 \right)$$
(8)

the above still not very useful, so **second attempt** is to make a little modification, where $a \to a$, and $b \to \eta b$

$$\|a - \eta b\|_{2}^{2} = \|a\|_{2}^{2} - 2\langle a, \eta b \rangle + \|\eta b\|_{2}^{2}$$

$$\implies \eta \langle a, b \rangle = \frac{\|a\|_{2}^{2} + \|\eta b\|_{2}^{2} - \|a - \eta b\|_{2}^{2}}{2}$$

$$\implies \langle a, b \rangle = \frac{\|a\|_{2}^{2} + \|\eta b\|_{2}^{2} - \|a - \eta b\|_{2}^{2}}{2\eta}$$
(9)

instead, i.e., $a = x_t - x^*$, and $\eta b = \eta \nabla f(x_t)$, brings nice cancellation:

$$f(x_{t+1}) \leq f(x^*) + \frac{1}{2\eta} \Big(\|x_t - x^*\|_2^2 + \|\eta \nabla f(x_t)\|_2^2 - \|x_t - x^* - \eta \nabla f(x_t)\|_2^2 - \|\eta \nabla f(x_t)\|_2^2 \Big)$$

$$= f(x^*) + \frac{1}{2\eta} \Big(\|x_t - x^*\|_2^2 - \|x_t - x^* - \eta \nabla f(x_t)\|_2^2 \Big)$$

$$= f(x^*) + \frac{1}{2\eta} \Big(\|x_t - x^*\|_2^2 - \|\underbrace{x_t - \eta \nabla f(x_t)}_{x_{t+1}} - x^*\|_2^2 \Big)$$

$$\implies f(x_{t+1}) - f(x^*) = \frac{1}{2\eta} \Big(\|x_t - x^*\|_2^2 - \|\underbrace{x_t - \eta \nabla f(x_t)}_{x_{t+1}} - x^*\|_2^2 \Big)$$

$$(10)$$

finally:

$$\epsilon \equiv f(x_T) - f(x^*) \le \frac{1}{T} \sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*) = \frac{1}{T} \sum_{t=1}^{T-1} \frac{1}{2\eta} \Big(\|x_t - x^*\|_2^2 - \|x_{t+1} - x^*\|_2^2 \Big)$$

$$= \frac{1}{T} \frac{1}{2\eta} \Big(\|x_0 - x^*\|_2^2 - \|x_T - x^*\|_2^2 \Big)$$
(11)

QUESTION: why can we conclude $f(x_T) - f(x^*) \le \frac{1}{T} \sum_{t=0}^{T-1} f(x_{t+1}) - f(x^*)$?

2 what concentration inequality is about?

imagine we have an "exact" (but un-achievable) bound, i.e., concentration equality

$$\Pr(X > \epsilon) = \beta$$
 or
$$\Pr(X < \epsilon) = 1 - \beta$$
 or (12)

then, let's look at concentration inequality:

3 To bound a positive random variable: Markov Inequality

Theorem 3 if X has support in \mathbb{R}^+ :

$$\Pr(X \ge s) \le \frac{\mathbb{E}(X)}{s} \tag{13}$$

proof for this can be understood by:

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x p(x) \, \mathrm{d}x = \int_{0}^{\infty} x p(x) \, \mathrm{d}x \quad \text{since } x > 0$$

$$= \int_{0}^{s} x p(x) \, \mathrm{d}x + \int_{s}^{\infty} x p(x) \, \mathrm{d}x \quad \text{pick arbitrary bound } s$$

$$\geq \int_{s}^{\infty} x p(x) \, \mathrm{d}x \quad x > 0 \implies \int_{0}^{s} x p(x) \, \mathrm{d}x > 0$$

$$\geq \int_{s}^{\infty} s p(x) \, \mathrm{d}x$$

$$= s \int_{s}^{\infty} p(x) \, \mathrm{d}x$$

$$= s \Pr(X \geq s)$$

$$\implies \Pr(X \geq s) \leq \frac{\mathbb{E}(X)}{s}$$
(14)

3.1 second proof

when
$$X < a : \mathbb{1}_{(X \ge a)} = 0 \implies a\mathbb{1}_{(X \ge a)} = \underbrace{0 \le X}_{\text{due to support of } X \ge 0}$$
when $X \ge a : \mathbb{1}_{(X \ge a)} = 1 \implies a\mathbb{1}_{(X \ge a)} = \underbrace{a \le X}_{\text{due to condition } (X \ge a)}$
(15)

in both cases, we have: $a\mathbbm{1}_{(X\geq a)}\leq X$, then:

$$\begin{split} a\mathbbm{1}_{(X\geq a)} & \leq X \\ \Longrightarrow \mathbb{E}\big[a\mathbbm{1}_{(X\geq a)}\big] & \leq \mathbb{E}[X] \\ \Longrightarrow a\mathbb{E}\big[\mathbbm{1}_{(X\geq a)}\big] & \leq \mathbb{E}[X] \\ \Longrightarrow a\Pr(X\geq a) & \leq \mathbb{E}[X] \\ & \text{think } \mathbbm{1}_A \text{ is Bernoulli R.V. with parameter } \Pr(A) \implies \mathbb{E}[\mathbbm{1}_A] & = \Pr(A) \\ \Longrightarrow \mathbb{E}[X] & \geq \frac{\Pr(X\geq a)}{a} \end{split} \tag{16}$$

4 Chebyshev's inequality

Chebyshev's inequality is the absolute version of Tail bound, as oppose to Chernoff bound (without absolute value):

$$\Pr(|X - \mathbb{E}(X)| \ge \epsilon) = \Pr(X - \mathbb{E}(X))^2 \ge \epsilon^2)$$

$$\le \frac{\mathbb{E}[(X - \mathbb{E}(X))^2]}{\epsilon^2}$$

$$= \frac{\operatorname{Var}(X)}{\epsilon^2}$$
(17)

4.1 Useful Fact

- 1. $\Pr(|X \mathbb{E}(X)| \ge \epsilon) = \Pr(X \mathbb{E}(X))^2 \ge \epsilon^2$, so you do not need to deal with $|\cdot|$. This fact can be used generically.
- 2. Although it's obvious, but only if you can prove symmetry, i.e.,:

$$\Pr(X - \mathbb{E}[X]) \ge \epsilon) \le C$$

$$\Pr(\mathbb{E}[X] - X) < -\epsilon) \le C$$
(18)

then you can claim:

$$\Pr(|X - \mathbb{E}(X)| \ge \epsilon) \le 2C$$
 (19)

4.2 alternative expressions of Chebyshev's inequality

$$\Pr(|X - \mathbb{E}(X)| \ge \epsilon) \le \frac{\operatorname{Var}(X)}{\epsilon^2}$$

$$\implies \Pr\left(\left|\frac{X - \mathbb{E}(X)}{\sigma(X)}\right| \ge \epsilon\right) \le \frac{1}{\epsilon^2} \quad \text{standardize R.V, s.t. its variance is 1}$$

$$\implies \Pr\left(\left|X - \mathbb{E}(X)\right| \ge \epsilon \sigma(X)\right) \le \frac{1}{\epsilon^2}$$

4.3 application of Chebyshev's inequality

we can use it to derive weak law of large number:

$$\forall_{\epsilon>0} \lim_{n \to \infty} \Pr(|\bar{X}_n - \mu| \le \epsilon) = 1 \tag{21}$$

this means that $\bar{X}_n \stackrel{p}{\to} \mu$, as $n \to \infty$, i.e., \bar{X}_n converge in probability to μ as $n \to \infty$

$$\operatorname{Var}(\bar{X}) = \operatorname{Var}\left(\frac{X_1 + X_2 + \dots + X_n}{n}\right)$$

$$= \left(\frac{1}{n}\right)^2 \operatorname{var}(X_1 + X_2 + \dots + X_n)$$

$$= \left(\frac{1}{n}\right)^2 \left(\sigma^2 + \sigma^2 + \dots + \sigma^2\right) \qquad \text{(since the } X_i\text{'s are independent)}$$

$$= \left(\frac{1}{n}\right)^2 n\sigma^2 = \frac{\sigma^2}{n}$$

using Chebyshev's inequality, let:

$$\Pr(|X - \mathbb{E}(X)| \ge \epsilon) \le \frac{\operatorname{Var}(X)}{\epsilon^2}$$

$$\implies \Pr(|\bar{X}_n - \mathbb{E}(\bar{X})| \ge \epsilon) \le \frac{\frac{\sigma^2}{n}}{\epsilon^2} \quad \text{sub } \operatorname{Var}(X) \to \frac{\sigma^2}{n}$$

$$= \frac{\sigma^2}{n\epsilon^2}$$
(23)

this means that $\bar{X}_n \stackrel{p}{\to} \mathbb{E}(\bar{X})$, as $n \to \infty$, i.e., \bar{X}_n converge in probability to $\mathbb{E}(\bar{X})$ as $n \to \infty$ note that the tail probability $\Pr(|X - \mathbb{E}(X)| \ge \epsilon)$ is decaying $O(\frac{1}{n})$ so it's actually quite slow.

5 Different types of Convergence

$$X_n \xrightarrow{\text{a.s.}} X \implies X_n \xrightarrow{\text{p}} X \implies X_n \xrightarrow{\text{d}} X$$
 (24)

5.1 Convergence in probability

these are equivalent:

$$X_{n} \xrightarrow{\mathbb{P}} X$$

$$\lim_{n \to \infty} \Pr(|X_{n} - X| \le \epsilon) = 1, \quad \forall \epsilon$$

$$\forall \epsilon, \delta \quad \exists N_{\epsilon, \delta} \quad \text{s.t. } P(|X_{n} - X| \ge \epsilon) \le \delta \quad \forall n > N_{\epsilon, \delta} \quad \text{note there is no limit}$$

$$X_{n} = o_{n}(1)$$

$$(25)$$

5.2 Example of $X_n \xrightarrow{d} X$: Central Limit Theorem

Theorem 4 if X_i (any arbitrary distribution) has finite non-zero variance σ^2 , for large n, \bar{X}_n approximately has a normal distribution with mean μ and standard deviation $\frac{\sigma}{\sqrt{n}}$

We can put **Theorem(4)** in equation:

$$\lim_{n \to \infty} \Pr\left(a \le \frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}} \le b\right) = \Phi(b) - \Phi(a)$$
 (26)

QUESTION: what type of convergence is above?

this is an example of $X_n \stackrel{d}{\to} X$: means that the limit of CDF of $\frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}}$ must be equal that of Gaussian, for any interval (a,b):

5.3 Show CLT implies WLLN

Let $a=-\frac{c}{\sigma}$ and $b=\frac{c}{\sigma}$, and use Eq.(26)

$$\lim_{n \to \infty} \Pr\left(-\frac{c}{\sigma} \le \frac{\bar{X}_n - \mu}{\sigma/\sqrt{n}} \le \frac{c}{\sigma}\right) = \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$$

$$\lim_{n \to \infty} \Pr\left(-c \le \sqrt{n}(\bar{X}_n - \mu) \le c\right) = \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$$

$$\lim_{n \to \infty} \Pr\left(-\frac{c}{\sqrt{n}} \le \bar{X}_n - \mu \le \frac{c}{\sqrt{n}}\right) = \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$$

$$\lim_{n \to \infty} \Pr\left(|\bar{X}_n - \mu| \le \frac{c}{\sqrt{n}}\right) = \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$$

$$(27)$$

think about the above: When n is small, probability for $\bar{X}_n - \mu$ to fall between $\left(\frac{-c}{\sqrt{n}}, \frac{-c}{\sqrt{n}}\right)$ may be less than $\Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right)$

1. As n becomes larger, we have a threshold $N_{\epsilon,\delta}$ such that, $\forall n>N_{\epsilon,\delta}$:

$$\Pr\left(\left|\bar{X}_n - \mu\right| \le \frac{c}{\sqrt{n}}\right) \ge \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right) - \frac{\delta}{2} \tag{28}$$

2. $\forall n \geq N_{\epsilon,\delta} \implies \frac{c}{\sqrt{n}} \leq \frac{c}{\sqrt{N}} \leq \epsilon$, and c > 0 is not arbitrary, we can always select c such that:

$$\Phi\left(-\frac{c}{\sigma}\right) \le \frac{\delta}{4} \tag{29}$$

$$\Pr\left(\left|\bar{X}_{n}-\mu\right| \leq \epsilon\right) \geq \Pr\left(\left|\bar{X}_{n}-\mu\right| \leq \frac{c}{\sqrt{n}}\right) \quad \text{LHS is looser bound}$$

$$\geq \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right) - \frac{\delta}{2}$$

$$\geq 1 - \frac{2\delta}{4} - \frac{\delta}{2} \quad \text{QUESTION: how may you derive this?}$$

$$= 1 - \delta$$
(30)

for symmetric pdf:

$$\begin{split} \Phi\left(\frac{c}{\sigma}\right) + \Phi\left(-\frac{c}{\sigma}\right) &= 1\\ \implies \Phi\left(\frac{c}{\sigma}\right) &= 1 - \Phi\left(-\frac{c}{\sigma}\right)\\ \Phi\left(\frac{c}{\sigma}\right) - \Phi\left(-\frac{c}{\sigma}\right) &= 1 - 2\Phi\left(-\frac{c}{\sigma}\right)\\ &\geq 1 - \frac{\delta}{2} \quad \text{using } \Phi\left(-\frac{c}{\sigma}\right) \leq \frac{\delta}{4} \end{split} \tag{31}$$

QUESTION: what if we change the relationship between c and δ to be $\Phi\left(-\frac{c}{\sigma}\right) \leq \frac{\delta}{3}$ instead?

5.3.1 explain the arbitrary choice of ϵ and δ

$$\forall \varepsilon, \delta \quad \exists N_{\varepsilon, \delta} \quad \text{s.t. } P(|X_n| \ge \epsilon) \le \delta \quad \forall n > N_{\varepsilon, \delta}$$
 (32)

$$\delta \to 0 \implies c \to \text{large} \quad \text{as } \Phi\left(-\frac{c}{\sigma}\right) \le \frac{\delta}{4}$$
 $\epsilon \to 0 \implies n \to \text{large} \quad \text{as } \frac{c}{\sqrt{n}} \le \epsilon$ (33)

note that as expected, δ is not computed as a function of ϵ . the two are obtained independently, via changing value of c, n, (the special case is not just n)

6 Moment Generation Function

Introduction to MGF

6.1 Using MGF to prove Central Limit Theorem

Theorem 5 Let X_1, \ldots, X_n be i.i.d R.V with $\mathbb{E}[X_k] = \mu$ and $Var(X_k) = \sigma^2 \leq \infty$, and $\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i$, then:

$$\sqrt{n} \left(\bar{X} - \mu \right) \stackrel{d}{\to} \mathcal{N}(0, \sigma^2)$$

$$\implies \sqrt{n} \left(\frac{\bar{X} - \mu}{\sigma} \right) \stackrel{d}{\to} \mathcal{N}(0, 1)$$
(34)

note μ and σ refer to a single R.V.

note that $X_n \stackrel{d}{\to} X$ means convergence in distribution, i.e.,

$$\lim_{n \to \infty} \Pr_n(X_n \le x) = \Pr(X \le x)$$
(35)

in words, as n goes to infinity, CDF of X_n converge to that of the X

6.1.1 proof

QUESTION: How do you proof convergence by distribution via MGF? if we can prove:

$$\begin{aligned} \text{MGF}_{\lim_{n \to \infty} \sqrt{n} \left(\frac{\bar{X} - \mu}{\sigma} \right)}(\lambda) &= \text{MGF}_{X_i \sim \mathcal{N}(0, 1)}(\lambda) \\ &= \exp \left(\frac{\lambda^2}{2} \right) \end{aligned} \tag{36}$$

we begin, to remove notation clarity, we remove $\lim_{n\to\infty}$:

$$\begin{aligned} \operatorname{MGF}_{\sqrt{n}\left(\frac{\bar{X}-\mu}{\sigma}\right)}(\lambda) &= \mathbb{E}\Big[\exp^{\lambda\left(\frac{\sqrt{n}}{\sigma}(\bar{X}-\mu)\right)}\Big] \\ &= \operatorname{MGF}_{\left(\bar{X}-\mu\right)}\left(\frac{\lambda\sqrt{n}}{\sigma}\right) \\ &= \operatorname{MGF}_{\left(\frac{\sum_{i=1}^{n}X_{i}-\mu}{n}\right)}\left(\frac{\lambda\sqrt{n}}{\sigma}\right) \\ &= \operatorname{MGF}_{\left(\sum_{i=1}^{n}(X_{i}-\mu)\right)}\left(\frac{\lambda}{\sigma\sqrt{n}}\right) \\ &= \left(\operatorname{MGF}_{\left(X_{i}-\mu\right)}\left(\frac{\lambda}{\sigma\sqrt{n}}\right)\right)^{n} \quad \text{property of MGF} \end{aligned}$$
(37)

so we use Taylor approximation of $\mathrm{MGF}_{(X_i-\mu)}\Big(\frac{\lambda}{\sigma\sqrt{n}}\Big)$ at $\lambda_0=0$. We need to use Taylor expansion here, as we are not after a specific moment.

$$\mathbb{E}\Big[f_{\lambda}(0) + \lambda f_{\lambda}'(0) + \frac{1}{2!}\lambda^{2}f_{\lambda}''(0) + \frac{1}{3!}\lambda^{3}f_{\lambda}'''(0) + O(\cdot)\Big] \\
= \mathbb{E}\Big[1 + \frac{\lambda}{\sigma\sqrt{n}}(X_{i} - \mu) + \frac{\lambda^{2}}{2\sigma^{2}n}(X_{i} - \mu)^{2} + \frac{\lambda^{3}}{3!\sigma^{2}n^{3/2}}(X_{i} - \mu)^{3}O(\cdot)\Big] \\
= 1 + \frac{\lambda}{\sigma\sqrt{n}}\underbrace{\mathbb{E}\Big[(X_{i} - \mu)\Big]}_{=0} + \frac{\lambda^{2}}{2\sigma^{2}n}\underbrace{\mathbb{E}\Big[(X_{i} - \mu)^{2}\Big]}_{\sigma^{2}} + \frac{\lambda^{3}}{3!\sigma^{2}n^{3/2}}\mathbb{E}\Big[(X_{i} - \mu)^{3}\Big] + O(\cdot) \tag{38}$$

$$= 1 + \frac{\lambda^{2}}{2n} + O(\cdot)$$

taking limit and higher order terms will disappear as faster as n in denominator, and also substitute $X_i \to \bar{X}$:

$$\lim_{n \to \infty} \mathsf{MGF}_{(\bar{X} - \mu)} \left(\frac{\lambda}{\sigma \sqrt{n}} \right)$$

$$= \lim_{n \to \infty} \left(1 + \frac{\lambda^2}{2n} \right)^n$$

$$= \exp\left(\frac{\lambda^2}{2} \right) \quad \lim_{n \to \infty} \left(1 + \frac{x}{n} \right)^n = \exp(x)$$
(39)

QUESTION: just for fun: let's try $X_i \sim \mathcal{N}(\mu, \sigma^2)$, and MGF of general 1-D Gaussian is $\exp^{\lambda \mu + \frac{1}{2}\sigma^2 \lambda^2}$ using Eq.(37):

$$\begin{split} \mathrm{MGF}_{\sqrt{n}\left(\frac{\bar{X}-\mu}{\sigma}\right)}(\lambda) &= \left(\mathrm{MGF}_{(X_i-\mu)}\left(\frac{\lambda}{\sigma\sqrt{n}}\right)\right)^n \quad \text{property of MGF} \\ &= \left(\exp^{\frac{\sigma^2\left(\frac{\lambda}{\sigma\sqrt{n}}\right)^2}{2}}\right)^n \quad \text{using MGF of Gaussian } \exp^{\lambda\mu+\frac{1}{2}\sigma^2\lambda^2} \\ &= \left(\exp^{\left(\frac{\lambda^2}{2n}\right)}\right)^n \\ &= \exp^{\left(\frac{\lambda^2}{2}\right)} \end{split}$$

note that there is no need to even take $\lim_{n \to \infty}$

7 references

in this tutorial, I have paraphrased a number of existing courses and notes, I encourage people to see the original notes too.

- https://engineering.purdue.edu/ChanGroup/ECE645Notes/StudentLecture04. pdf
- 2. http://www.dklevine.com/archive/strong-law.pdf
- 3. various Wikipedia pages