Machine Learning and Neural Networks III (MATH3431)

Epiphany term

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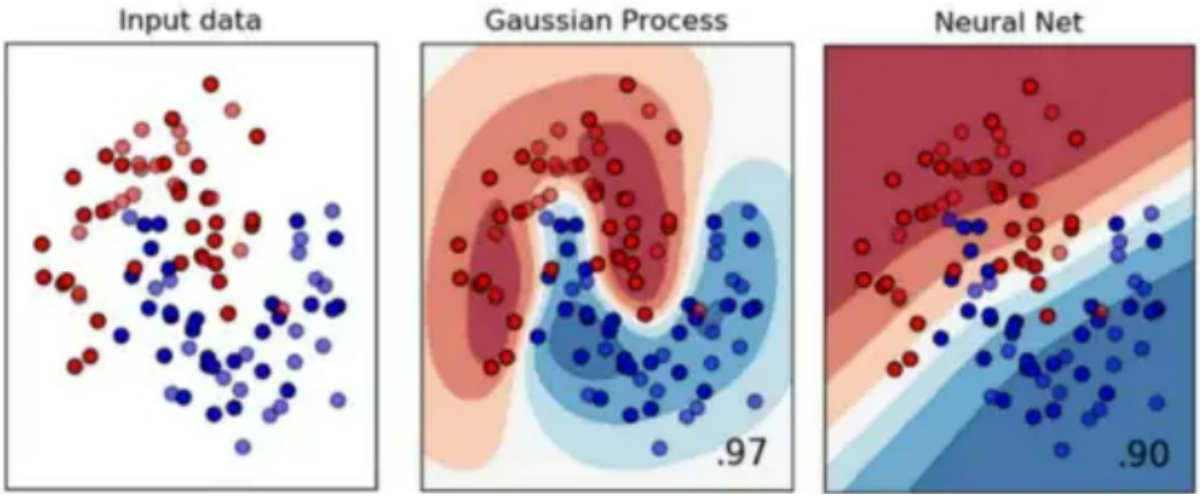
Concepts

- Convex learning problems
- Stochastic learning
- Support vector machines
- Artificial neural networks
- Kernel methods
- Gaussian process regression



Reading list

These lecture Handouts have been derived based on the above reading list.

Main texts:

- Bishop, C. M. (2006). Pattern recognition and machine learning. New York: Springer.
  - It is a classical textbook in machine learning (ML) methods. It discusses all the concepts introduced in the course (not necessarily in the same depth). It is one of the main textbooks in the module. The level on difficulty is easy.
  - Students who wish to have a textbook covering traditional concepts in machine learning are suggested to get a copy of this textbook. It is available online from the Microsoft's website `https://www.microsoft.com/en-us/research/publication/pattern-recogniti`
- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
  - It has several elements of theory about machine learning algorithms. It is one of the main textbooks in the module. The level on difficulty is advanced as it requires moderate knowledge of maths.
- Bishop, C. M. (1995). Neural networks for pattern recognition. Oxford university press.
  - It is a classical textbook about 'traditional' artificial neural networks (ANN). It is very comprehensive (compared to others) and it goes deep enough for the module although it may be a bit outdated. It is one of the main textbooks in the module for ANN. The level on difficulty is moderate.

Supplementary textbooks:

- Ripley, B. D. (2007). Pattern recognition and neural networks. Cambridge university press.
  - A classical textbook in artificial neural networks (ANN) that also covers other machine learning concepts. It contains interesting theory about ANN.
  - It is suggested to be used as a supplementary reading for neural networks as it contains a few interesting theoretical results. The level on difficulty is moderate.
- Williams, C. K., & Rasmussen, C. E. (2006). Gaussian processes for machine learning (Vol. 2, No. 3, p. 4). Cambridge, MA: MIT press.

  - A classic book in Gaussian process regression (GPR) that covers the material we will discuss in the course about GPR. It can be used as a companion textbook with that of (Bishop, C. M., 2006). The level on difficulty is easy.

- Murphy, K. P. (2012). Machine learning: a probabilistic perspective. MIT press.

  - A popular textbook in machine learning methods. It discusses all the concepts introduced in the module. It focuses more on the probabilistic/Bayesian framework but not with great detail. It can be used as a comparison textbook for brief reading about ML methods just to see another perspective than that in (Bishop, C. M., 2006). The level on difficulty is easy.

- Murphy, K. P. (2022). Probabilistic machine learning: an introduction. MIT press.

  - A textbook in machine learning methods. It covers a smaller number of ML concepts than (Murphy, K. P., 2012) but it contains more fancy/popular topics such as deep learning ideas. It is suggested to be used in the same manner as (Murphy, K. P., 2012). The level on difficulty is easy.

- Barber, D. (2012). Bayesian reasoning and machine learning. Cambridge University Press.

  - A textbook in machine learning methods from a Bayesian point of view. It discusses all the concepts introduced apart from ANN and stochastic gradient algorithms. It aims to be more 'statistical' than those of Murphy and Bishop. The level on difficulty is easy.

- Vapnik, V. (1999). The nature of statistical learning theory. Springer science & business media.

  - Important textbook in the statistical machine learning theory. To have have an in deep understanding about statistical learning, one has to read it together with the textbook of Shalev-Shwartz, S., & Ben-David, S. (2014)

- Devroye, L., Györfi, L., & Lugosi, G. (2013). A probabilistic theory of pattern recognition (Vol. 31). Springer Science & Business Media.

  - Theoretical aspects about machine learning algorithms. The level on difficulty is advanced as it requires moderate knowledge of probability.

Contents

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3. Handout 3: Learnability, and stability
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5. Handout 5: Stochastic gradient descent
6. Handout 6: Bayesian Learning via Stochastic gradient and Stochastic gradient Langevin dynamics

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

Handout 1: Machine learning –A recap on: definitions, notation, and formalism

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Aim. To get some definitions and set-up about the learning procedure; essentially to formalize what introduced in term 1.

Reading list & references:

- Bishop, C. M. (2006). Pattern recognition and machine learning. New York: Springer.
  - Ch. 1 Introduction
- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
  - Ch. 1 Introduction

1. General Introductions and loose definitions

Pattern recognition is the automated discovery of patterns and regularities in data $z \in \mathcal{Z}$. **Machine learning (ML)** are statistical procedures for building and understanding probabilistic methods that 'learn'. **ML algorithms** $\mathfrak{A}$ build a (probabilistic/deterministic) model able to make predictions or decisions with minimum human interference and can be used for pattern recognition. **Learning** (or training, estimation, fitting) is called the procedure where the ML model is tuned. **Training data** (or observations, sample data set, examples) is a set of observables $\{z_i \in \mathcal{Z}\}$ used to tune the parameters of the ML model. By $\mathcal{Z}$ we denote the examples (or observables) domain. **Test set** is a set of available examples/observables $\{z_i'\}$ (different than the training data) used to verify the performance of the ML model for a given a measure of success. **Measure of success** (or performance) is a quantity that indicates how bad the corresponding ML model or Algorithm performs (eg quantifies the failure/error), and can also be used for comparisons among different ML models; eg, **Risk function** or **Empirical Risk Function**. Two main problems in ML are the supervised learning (we will focus on this here) and the unsupervised learning.

Supervised learning problems involve applications where the training data $z \in \mathcal{Z}$ comprise examples of the input vectors $x \in \mathcal{X}$ along with their corresponding target vectors $y \in \mathcal{Y}$; i.e. $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. By $\mathcal{X}$ we denote the inputs (or instances) domain, and by $\mathcal{Y}$ we denote the target domain. **Classification problems** are those which aim to assign each input vector x to one of a finite number of discrete categories of y. **Regression problems** are those where the output y consists of one or more continuous variables. All in all, the learner wishes to discover an unknown pattern (i.e. functional relationship) between components $x \in \mathcal{X}$ that serves as inputs and components $y \in \mathcal{Y}$ that act as outputs; i.e. $x \longmapsto y$. Hence, $\mathcal{X}$ is the input domain, and $\mathcal{Y}$ is the output (or target) domain. The goal of learning is to discover a function which predicts (or help us make decisions about) $y \in \mathcal{Y}$ from $x \in \mathcal{X}$.

Unsupervised learning problems involve applications where the training data $z \in \mathcal{Z}$ consist of a set of input vectors $x \in \mathcal{X}$ without any corresponding target values ; i.e. $\mathcal{Z} = \mathcal{X}$. In clustering the goal is to discover groups of similar examples within the data of it is to discover groups of similar examples within the data.

2. (loose) Notation & definitions in learning

Definition 1. The learner's output is a function, $h : \mathcal{X} \to \mathcal{Y}$ which predicts $y \in \mathcal{Y}$ from $x \in \mathcal{X}$. It is also called Hypothesis, prediction rule, predictor, or classifier.

Notation 2. We often denote the set of hypothesis as $\mathcal{H}$; i.e. $h \in \mathcal{H}$.

Example 3. (Linear Regression)[1] Consider the regression problem where the goal is to learn the mapping $x \to y$ where $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and $y \in \mathcal{Y} \subseteq \mathbb{R}$. A hypothesis is a linear function $h : \mathcal{X} \to \mathcal{Y}$ (that learner wishes to learn) with $h(x) = \langle w, x \rangle$ approximating the mapping $x \to y$. The hypothesis set $\mathcal{H} = \left\{ x \to \langle w, x \rangle : w \in \mathbb{R}^d \right\}$.

Example 4. (Binary Classification) Consider the classification problem where the goal is to learn the mapping $x \to y$ where $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and $y \in \mathcal{Y}\{-1, +1\}$. A hypothesis can be a function $h : \mathcal{X} \to \mathcal{Y}$ with $h(x) = \text{sign}(\langle w, x \rangle)$ approximating the mapping $x \to y$. The hypothesis set $\mathcal{H} = \left\{ x \to \text{sign}(\langle w, x \rangle) : w \in \mathbb{R}^d \right\}$.

Definition 5. Training data set $\mathcal{S}$ of size m is any finite sequence of pairs $(z_i = (x_i, y_i) ; i = 1, ..., m)$ in $\mathcal{X} \times \mathcal{Y}$; i.e. $\mathcal{S} = \{(x_i, y_i) ; i = 1, ..., m\}$. This is the information that the learner has assess.

Definition 6. Data generation model $g(\cdot)$ is the probability distribution over $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, unknown to the learner that has generated the data. E.g. $z \sim g$.

Definition 7. We denote as $\mathfrak{A}(\mathcal{S})$ the hypothesis (outcome) that a learning algorithm $\mathfrak{A}$ returns given training sample S.

Definition 8. (Loss function) Given any set of hypothesis $\mathcal{H}$ and some domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, a loss function $\ell(\cdot)$ is any function $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}_+$. Loss function $\ell(h, z)$ for $h \in \mathcal{H}$ and $z \in \mathcal{Z}$ is specified according to the purpose the machine learning algorithm. It reflects how the "error" is quantified for a given hypothesis h and a given example z. The rule is "the greater the error the greater the value of the loss".

Example 9. (Cont. Example 3) In regression problems $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ and $\mathcal{Y} \subset \mathbb{R}$ is uncountable, a potential loss function is

$$\ell_{\text{sq}}(h, (x, y)) = (h(x) - y)^2$$

Example 10. (Cont. Example 4) In binary classification problems with hypothesis $h : \mathcal{X} \to \mathcal{Y}$ where $\mathcal{Y} = \{0, 1\}$ is discrete, a loss function can be

$$\ell_{0-1}(h, (x, y)) = 1(h(x) \neq y),$$

[1] $\langle w, x \rangle = w^\top x$

Definition 11. (Risk function) The risk function $R_g(h)$ of h is the expected loss of the hypothesis $h \in \mathcal{H}$, w.r.t. the data generation model (which is a probability distribution) g over domain Z; i.e.

$$R_g(h) = \mathrm{E}_{z\sim g}(\ell(h,z)) \tag{2.1}$$

Remark 12. In learning, an ideal way to obtain an optimal predictor h^* is to compute the minimizer of the risk; i.e.

$$h^* = \arg\min_{\forall h}(R_g(h)) \tag{2.2}$$

Example 13. (Cont. Ex. 9) The risk function is $R_g(h) = \mathrm{E}_{z\sim g}(h(x)-y)^2$, and it measures the quality of the hypothesis function $h : \mathcal{X} \to \mathcal{Y}$, (or equiv. the validity of the class of hypotheses $\mathcal{H}$) against the data generating model g, as the expected square difference between the predicted values form h and the true target values y at every x.

Note 14. Computing the risk minimizer may be practically challenging due to the integration w.r.t. the unknown data generation model g involved in the expectation (2.1). Sub-optimally, one may use the Empirical risk function instead of the Risk function in (2.2).

Definition 15. (Empirical risk function) The Empirical Risk Function (ERF) $\hat{R}_S(h)$ of h is the expectation of loss of h over a given sample $S = (z_1, ..., z_m) \in \mathcal{Z}^m$; i.e.

$$\hat{R}_S(h) = \frac{1}{m}\sum_{i=1}^{m}\ell(h,z_i).$$

Remark 16. Given Empirical Risk Function (ERF) $\hat{R}_S(h)$ of h the optimal predictor h^* is the minimizer of the ERF; i.e.

$$h^* = \arg\min_{\forall h}\left(\hat{R}_S(h)\right) \tag{2.3}$$

Example 17. (Cont. Example 13) Given given sample $S = \{(x_i, y_i); i = 1, ..., m\}$ the empirical risk function is $\hat{R}_S(h) = \frac{1}{m}\sum_{i=1}^{m}(h(x_i)-y_i)^2$.

Example 18. (Cont. Example 10) Given given sample $S = \{(x_i, y_i); i = 1, ..., m\}$ the empirical risk function is $\hat{R}_S(h) = \frac{1}{m}\sum_{i=1}^{m}1(h(x_i) \neq y_i)$.

Remark 19. If the Hypothesis set $\mathcal{H}$ is a known parametric family of functions; i.e. $\mathcal{H} = \{h_w(\cdot); w \in \mathcal{W}\}$ parameterized by unknown $w \in \mathcal{W}$, then we can equivalently consider $\mathcal{H} = \{w \in \mathcal{W}\} = \mathcal{W}$ keeping in mind that the learner's output is restricted to $h_w(\cdot)$.

Example 20. Consider the multiple linear regression problem with regressors $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and response $y \in \mathcal{Y} \subseteq \mathbb{R}$. Because it involves only linear functions as predictors $h_w(x) = \langle w, x\rangle$, we could consider a hypothesis class $\mathcal{H} = \left\{w \in \mathbb{R}^d\right\} = \mathbb{R}^d$ and loss function loss $\ell(w,(x,y)) = (\langle w, x\rangle - y)^2$ for computational simplicity. The latter will be mainly used.

Example 21. Consider a learning problem where the true data generation distribution (unknown to the learner) is $g(z)$, the statistical model (known to the learner) is given by a sampling distribution

$f_\theta(y) := f(y|\theta)$ labeled by an unknown parameter θ. The goal is to learn θ. If we assume loss function

$$\ell(\theta, z) = \log\left(\frac{g(z)}{f_\theta(z)}\right)$$

then the risk is

$$R_g(\theta) = \mathrm{E}_{z\sim g}\left(\log\left(\frac{g(z)}{f_\theta(z)}\right)\right) = \mathrm{E}_{z\sim g}(\log(g(z))) - \mathrm{E}_{z\sim g}(\log(f_\theta(z))) \tag{2.4}$$

whose minimizer is

$$\theta^* = \arg\min_{\forall\theta}(R_g(\theta)) = \arg\min_{\forall\theta}(\mathrm{E}_{z\sim g}(-\log(f_\theta(z))))$$

as the first term in (2.4) is constant. Note that in the Maximum Likelihood Estimation technique the MLE θ_{MLE} is the minimizer

$$\theta_{\mathrm{MLE}} = \arg\min_{\theta}\left(\frac{1}{m}\sum_{i=1}^{m}(-\log(f_\theta(z_i)))\right)$$

where $S = \{z_1, ..., z_m\}$ is an IID sample from g. Hence, MLE θ_{MLE} can be considered as the minimizer of the empirical risk $R_S(\theta) = \frac{1}{m}\sum_{i=1}^{m}(-\log(f_\theta(z_i)))$.

Definition 22. A learning problem with hypothesis class $\mathcal{H}$, examples domain $\mathcal{Z}$, and loss function ℓ may be denoted with a triplet $(\mathcal{H}, \mathcal{Z}, \ell)$.

Example 23. The standard multiple linear regression problem with regressors $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and response $y \in \mathcal{Y} \subseteq \mathbb{R}$, is a learning problem with examples domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y} = \mathbb{R}^{d+1}$, hypothesis class $\mathcal{H} = \left\{x \to \langle w, x\rangle : w \in \mathbb{R}^d\right\}$, and loss function $\ell_{\mathrm{sq}}(h, (x, y)) = (h(x) - y)^2$.

Appendix A. Useful things

Below are some standard notation used as default in the notes except in cases that is defined otherwise.

- $q-$norm: When $x \in \mathbb{R}^d$ $\|x\|_q := \left(\sum_{j=1}^{d} x_j^q\right)^{1/q}$
- Manhattan norm: When $x \in \mathbb{R}^d$ $\|x\|_1 := \sum_{j=1}^{d} |x_j|$
- Euclidean norm: When $x \in \mathbb{R}^d$ $\|x\|_2 := \sqrt{\sum_{j=1}^{d} x_j^2}$. When $\|\cdot\|$ we will assume the Euclidean norm.
- Infinity norm or maximum norm: $\|x\|_\infty := \max_{\forall j} |x_j|$
- Inner product of x , y: If $x, y \in \mathbb{R}^d$ then $\langle x, y\rangle = x^\top y$. So $\langle x, x\rangle = \|x\|^2$

Also some standard formulas.

- Jensens' inequality: If If $x \in \mathbb{R}^d$ and $f : \mathbb{R}^d \to \mathbb{R}$ then

$$\begin{cases} f(\mathrm{E}(x)) \le \mathrm{E}(f(x)) & \text{if } f \text{ is convex} \\ f(\mathrm{E}(x)) \ge \mathrm{E}(f(x)) & \text{if } f \text{ is concave} \end{cases}$$

- Cauchy–Schwarz inequality: If $x, y \in \mathbb{R}^d$ then $|\langle x, y\rangle|^2 \le \langle x, x\rangle\langle y, y\rangle$ equiv. $|\langle x, y\rangle| \le \|x\|\,\|y\|$.

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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

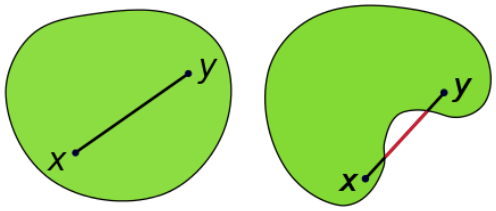
Note 1. We introduce concepts of convexity and smoothness that facilitate the analysis and understanding of the learning problems and their solutions that we will discuss (eg stochastic gradient descent, SVM) later on. Also learning problems with such characteristics can be learned more efficiently.

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 $\alpha \in [0, 1]$

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

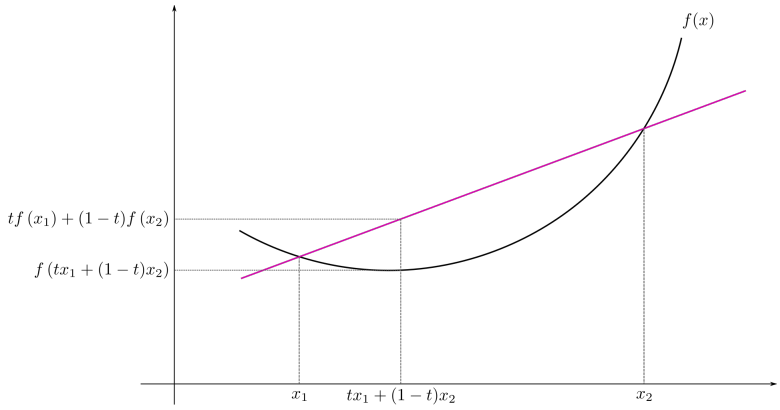


FIGURE 2.2. A convex function

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

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

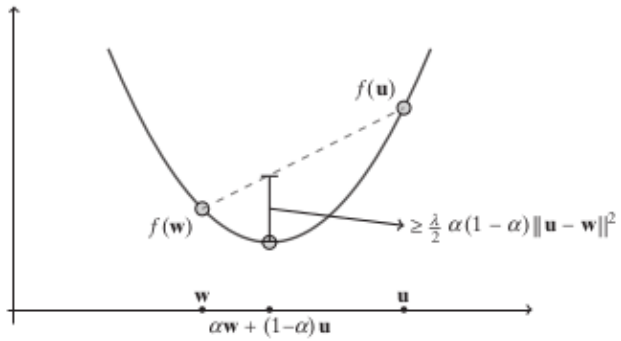


FIGURE 7.1. Strongly convex function

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. □

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

Handout 3: Learnability and stability in learning problems

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Aim. To introduce concepts PAC, fitting vs stability trade off, stability, and their implementation in regularization problems and convex problems.

Reading list & references:

- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
  - Ch. 2, 3, 13
- Vapnik, V. (2000). The nature of statistical learning theory. Springer science & business media. (too advanced)

1. Learnable Probably Approximately Correct (PAC) Learning

Note 1. We formally define the broad learning problem we will work on.

Note 2. Learning algorithms $\mathfrak{A}$ use training data sets $\mathcal{S}$ which may miss characteristics of the unknown data-generating process g. Essentially, approximations (aka errors) are inevitable; some characteristics of data generating process g will be missed even if we use a very representative training set $\mathcal{S}$. We cannot hope that the learning algorithm will find a hypothesis whose error is smaller than the minimal possible error.

Note 3. The PAC learning problem requires no prior assumptions about the data-generating process g. It requires that the learning algorithm $\mathfrak{A}$ will find a predictor $\mathfrak{A}(\mathcal{S})$ whose error is not much larger than the best possible error of a predictor in some given benchmark hypothesis class. So essentially, in practice, the researcher's effort falls on the hypothesis class $\mathcal{H}$.

Definition 4. (Agnostic PAC Learnability for General Loss Functions) A hypothesis class $\mathcal{H}$ is agnostic PAC learnable with respect to a domain $\mathcal{Z}$ and a loss function $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}_+$, if there exist a function $m_{\mathcal{H}} : (0,1)^2 \to \mathbb{N}$ and a learning algorithm $\mathfrak{A}$ with the following property:

- for every $\epsilon \in (0,1)$, $\delta \in (0,1)$, and distribution g over $\mathcal{Z}$, when running algorithm $\mathfrak{A}$ given training set $\mathcal{S}_m = \{z_1, ..., z_m\}$ with $z_i \overset{\text{IID}}{\sim} g$ for $m \geq m_{\mathcal{H}}(\epsilon, \delta)$ then $\mathfrak{A}$ returns $\mathfrak{A}(\mathcal{S}) \in \mathcal{H}$ such as

$$\Pr_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}_m\right)\right) - \min_{h'\in\mathcal{H}}\left(R_g\left(h'\right)\right) \leq \epsilon\right) \geq 1-\delta \tag{1.1}$$

Note 5. It may be easier to work with expectations: by using Markov inequality (1.1) becomes

$$\Pr_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}_m\right)\right) - \min_{h'\in\mathcal{H}}\left(R_g\left(h'\right)\right) \leq \epsilon\right) \geq 1 - \frac{1}{\epsilon}\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}_m\right)\right) - \min_{h'\in\mathcal{H}}\left(R_g\left(h'\right)\right)\right) \tag{1.2}$$

and hence we need to work with expectations and bounded above.

Hint: Markov inequality $\Pr(X \geq a) \leq \frac{1}{a}\mathrm{E}(X)$ for $X > 0$.

Remark 6. About 1.2: The accuracy parameter ϵ determines how far the output rule $\mathfrak{A}(\mathcal{S}_m)$ of $\mathfrak{A}$ can be from the optimal one (this corresponds to the 'approximately correct'). The confidence parameter δ indicates how likely the classifier is to meet that accuracy requirement (corresponds to the "probably" part of "PAC").

2. Analysis of the risk based on the trade-off fitting vs stability

Note 7. Let $R^* = \min_{\forall h}(R(h))$ be an ideal/optimal (hence minimum) Risk, and $\mathfrak{A}(\mathcal{S})$ the learning rule from a learning algorithm $\mathfrak{A}$ trained against dataset $\mathcal{S}$. The Risk of a learning algorithm $\mathfrak{A}$ can be decomposed as

$$R_g(\mathfrak{A}(\mathcal{S})) - R^* = \hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S})) - R^* + \underbrace{R_g(\mathfrak{A}(\mathcal{S})) - \hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S}))}_{\text{over-fitting}} \tag{2.1}$$

Note 8. Over-fitting can be represented by $R_g(\mathfrak{A}(\mathcal{S})) - \hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S}))$. However, $\hat{R}_{\mathcal{S}}(\cdot)$ is a random variable and, here, for our computational convenience, we focus on its expectation w.r.t. $\mathcal{S} \sim g$. Hence, we provide the following (arguable) definition for over-fitting on which we base our analysis.

Definition 9. For a learning algorithm $\mathfrak{A}$, as a measure of over-fitting we consider the expected difference between true Risk and empirical Risk

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g(\mathfrak{A}(\mathcal{S})) - \hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S}))\right) \tag{2.2}$$

Definition 10. We say that learning algorithm $\mathfrak{A}$ suffers from over-fitting when (2.2) is 'too' large.

Note 11. The expected Risk of a learning algorithm $\mathfrak{A}(\mathcal{S})$ can be decomposed as

$$\mathrm{E}_{\mathcal{S}\sim g}(R_g(\mathfrak{A}(\mathcal{S}))) = \underbrace{\mathrm{E}_{\mathcal{S}\sim g}\left(\hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S}))\right)}_{\text{(I)}} + \underbrace{\mathrm{E}_{\mathcal{S}\sim g}\left(R_g(\mathfrak{A}(\mathcal{S})) - \hat{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S}))\right)}_{\text{(II)}} \tag{2.3}$$

by applying expectations in (2.1) and ignoring R^*. (I) indicates how well $\mathfrak{A}(\mathcal{S})$ fits the training set $\mathcal{S}$, and (II) indicates the discrepancy between the true and empirical risks of $\mathfrak{A}(\mathcal{S})$. In Section 3, we argue that the over-fitting term (II) is directly related to a certain type of stability of $\mathfrak{A}(\mathcal{S})$.

Note 12. The following result connects the need for upper bounding (and minimizing this bound) the Expected Risk in (2.3) and PAC learning (Definition 4).

Proposition 13. *Let $\mathfrak{A}$ be a learning algorithm that guarantees the following:*

- *If $m \geq m_{\mathcal{H}}(\epsilon)$ then for every distribution g, it is*

$$E_{\mathcal{S}\sim g}(R_g(\mathfrak{A}(\mathcal{S}_m))) \leq \min_{h'\in\mathcal{H}}\left(R_g\left(h'\right)\right) + \epsilon$$

Then $\mathfrak{A}$ satisfies the PAC guarantee in Definition 4:

- *for every $\delta \in (0,1)$, if $m \geq m_{\mathcal{H}}(\epsilon\delta)$* then

$$\Pr_{\mathcal{S}\sim g}\left(R_g(\mathfrak{A}(\mathcal{S}_m)) - \min_{h'\in\mathcal{H}}\left(R_g\left(h'\right)\right) \leq \epsilon\right) \geq 1 - \delta$$

Proof. Let $\xi = R_g\left(\mathfrak{A}\left(\mathcal{S}_m\right)\right) - \min_{h' \in \mathcal{H}}\left(R_g\left(h'\right)\right)$. From Markov's inequality $\Pr\left(\xi \geq \mathrm{E}\left(\xi\right)/\delta\right) \leq \frac{1}{\mathrm{E}(\xi)/\delta}\mathrm{E}\left(\xi\right) = \delta$. Namely, $\Pr\left(\xi \leq \mathrm{E}\left(\xi\right)/\delta\right) = 1-\delta$. But it is given that if $m \geq m_{\mathcal{H}}\left((\epsilon\delta)\right)$ for every distribution g it is $\mathrm{E}\left(\xi\right) \leq (\epsilon\delta)$. So by substitution $\Pr\left(\xi \leq (\epsilon\delta)/\delta\right) = 1-\delta$ implies $\Pr\left(\xi \leq \epsilon\right) = 1-\delta$. Now substitute back ξ and we conclude the proof. □

Note 14. Hence, we aim to design a learning algorithm $\mathfrak{A}\left(\mathcal{S}\right)$ that both fits the training set and is stable; i.e, keep both (I) and (II) in (2.3) small. As seen later, in certain learning problems, there may be a trade-off between empirical risk term (I) and (II) in (2.3). Consequently, we aim to upper bound (2.3) by upper bounding (I) and (II) individually and decide which term we should benefit against the other to achieve a certain total bound.

3. Stability and its association with over-fitting

Notation 15. Consider a learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$. Let $\mathcal{S} = \{z_1, ..., z_m\}$ be a training sample, and $\mathfrak{A}$ be a learning algorithm with output $\mathfrak{A}\left(\mathcal{S}\right)$.

Note 16. It is reasonable to consider that a learning algorithm $\mathfrak{A}$ can be stable if a small change of the algorithm input does not change the algorithm output much. Mathematically formalizing this, we can say that if $\mathcal{S}^{(i)} = \{z_1, ..., z_{i-1}, z', z_{i+1}, ..., z_m\}$ is another training dataset equal to $\mathcal{S}$ but the ith element being replaced by another independent example $z' \sim g$, then a good learning algorithm $\mathfrak{A}$ would produce a small value of

$$\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right) \geq 0$$

Definition 17. A learning algorithm $\mathfrak{A}$ is **on-average-replace-one-stable** with rate a decreasing function $\epsilon : \mathbb{N} \to \mathbb{R}$ if for every distribution g

$$\mathrm{E}_{\substack{\mathcal{S} \sim g \\ z' \sim g, i \sim \mathrm{U}\{1,...,m\}}} \left(\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right)\right) \leq \epsilon\left(m\right) \tag{3.1}$$

Note 18. The following result demonstrates the direct association of stability and over-fitting as defined in Definitions 10 & 17.

Theorem 19. *For any learning algorithm* $\mathfrak{A}$ *it is*

$$E_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right) - \hat{R}_{\mathcal{D}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) = E_{\substack{\mathcal{S} \sim g,\, z' \sim g \\ i \sim U\{1,...,m\}}} \left(\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right)\right) \tag{3.2}$$

where g *is a distribution,* $\mathcal{S} = \{z_1, ..., z_m\}$ *and* $\mathcal{S}^{(i)} = \{z_1, ..., z_{i-1}, z', z_{i+1}, ..., z_m\}$ are *training datasets with* $z', z_1, ..., z_m \overset{\text{iid}}{\sim} g$.

Proof. As $z', z_1, ..., z_m \overset{\text{iid}}{\sim} g$, then for every i

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) = \mathrm{E}_{\substack{\mathcal{S} \sim g \\ z' \sim g}} \left(\ell\left(\mathfrak{A}\left(\mathcal{S}\right), z'\right)\right) = \mathrm{E}_{\substack{\mathcal{S} \sim g \\ z' \sim g}} \left(\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right)\right)$$

and

$$\mathrm{E}_{\mathcal{S}\sim g}\left(\hat{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right)=\mathrm{E}_{\substack{\mathcal{S}\sim g\\ i\sim U\{1,...,m\}}}\left(\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right),z_i\right)\right)$$

□

Note 20. Hence, we desire to design learning algorithms corresponding to as small as possible (3.2).

4. Implementation in regularized loss learning problems

Definition 21. A Regularized Loss Minimization (RLM) learning problem $(\mathcal{H},\mathcal{Z},\ell)$ with a regularization function $J:\mathcal{H}\to\mathbb{R}$ aims at a RLM learning rule that is the minimizer

$$h^*=\arg\min_{h\in\mathcal{H}}\left(\hat{R}_{\mathcal{S}}\left(h\right)+J\left(h\right)\right) \tag{4.1}$$

where $\hat{R}_{\mathcal{S}}\left(\cdot\right)=\frac{1}{m}\sum_{i=1}^{m}\ell\left(\cdot,z_i\right)$, and $\mathcal{S}=\{z_1,...,z_m\}\subset$ an IID training sample.

Remark 22. The motivation for considering the regularization function J in (4.1) is to: (1.) control complexity and (2.) improve stability; as we will see later.

Note 23. Here, we make our example more specific and narrow it to the Ridge RLM learning problem (could have been LASSO etc.).

Definition 24. The Ridge RLM learning problem $(\mathcal{H},\mathcal{Z},\ell)$, with $\mathcal{H}=\mathcal{W}\subset\mathbb{R}^d$, uses regularization function $J\left(w;\lambda\right)=\lambda\left\|w\right\|_2^2$ with $\lambda>0$, $w\in\mathcal{W}$ and produces learning rule

$$\mathfrak{A}\left(\mathcal{S}\right)=\arg\min_{w\in\mathcal{W}}\left(\hat{R}_{\mathcal{S}}\left(w\right)+\lambda\left\|w\right\|_2^2\right) \tag{4.2}$$

Note 25. Recall (Term 1) how the regularization function in Ridge RLM learning problem $(\mathcal{H},\mathcal{Z},\ell)$ penalizes complexity. Essentially, it implies a sequence of hypothesis $\mathcal{H}_1\subset\mathcal{H}_2\subset...$ with $\mathcal{H}_i=\left\{w\in\mathbb{R}^d:\left\|w\right\|_2<i\right\}$ due to duality of the corresponding minimization problem.

Note 26. Below, we will try to analyze the behavior of Ridge RLM learning rule (4.2) w.r.t. the Risk decomposition (2.3). In particular, to upper bounded w.r.t. the shrinkage term λ, training sample size m, and other characteristics.

4.1. Bounding the empirical risk (I) in (2.3).

Note 27. From (4.2), we have

$$\begin{aligned}\hat{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)&\leq\hat{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)+\lambda\left\|\mathfrak{A}\left(\mathcal{S}\right)\right\|_2^2\\&\leq\hat{R}_{\mathcal{S}}\left(w\right)+\lambda\left\|w\right\|_2^2;\quad\forall w\in\mathcal{W}\end{aligned}$$

and by taking expectations w.r.t. $\mathcal{S}$, it is

$$\mathrm{E}_{\mathcal{S}\sim g}\left(\hat{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right)\leq R_g\left(w\right)+\lambda\left\|w\right\|_2^2;\quad\forall w\in\mathcal{W} \tag{4.3}$$

because $\mathrm{E}_{\mathcal{S}\sim g}\left(\hat{R}_{\mathcal{S}}\left(\cdot\right)\right)=\frac{1}{m}\sum_{i=1}^{m}\mathrm{E}_{\mathcal{S}\sim g}\left(\ell\left(\cdot,z_i\right)\right)=R_g\left(\cdot\right)$.

Note 28. From (4.3), we observe that part (I) in the expected risk decomposition (2.3), (aka the upper bound of the expected empirical risk) increases with the regularization term $\lambda > 0$. (!!!) –Although anticipated, it did not start well.

4.2. **Bounding the empirical risk (II) in (2.3).**

Note 29. As we will see to bound (II) in (2.3) we will have to impose an additional condition on the behavior of loss function apart from convexity; e.g. Lipstchitzness.

Assumption 30. *The loss function $\ell(\cdot, z)$ in (4.2) is convex for any $z \in \mathcal{Z}$.*

Note 31. Let $\tilde{R}_{\mathcal{S}}(w) = \hat{R}_{\mathcal{S}}(w) + \lambda \|w\|_2^2$. $\tilde{R}_{\mathcal{S}}(\cdot)$ is 2λ-strongly convex as the sum of a convex function $\hat{R}_{\mathcal{S}}(\cdot)$ (Assumption 30) and a 2λ-strongly convex function $J(\cdot;\lambda) = \lambda \|\cdot\|_2^2$ (results directly from Definition 38 in Handout 2).

Fact 32. *(To be used in Note 33) If f is λ-strongly convex and u is a minimizer of f then for any w*

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

Note 33. Let $\mathfrak{A}(\mathcal{S})$ be the Ridge learning algorithm output minimizing (4.2). Because $\tilde{R}_{\mathcal{S}}(\cdot)$ is 2λ-strongly convex and $\mathfrak{A}(\mathcal{S})$ is its minimizer, according to Fact 32, for $\mathfrak{A}(\mathcal{S})$ and any $w \in \mathcal{W}$, it is

$$\tilde{R}_{\mathcal{S}}(w) - \tilde{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S})) \geq \lambda \|w - \mathfrak{A}(\mathcal{S})\|^2, \quad \forall w \in \mathcal{W} \tag{4.4}$$

Note 34. Also, for any $w, u \in \mathcal{W}$, it is

$$\begin{aligned}
\tilde{R}_{\mathcal{S}}(w) - \tilde{R}_{\mathcal{S}}(u) &= \left(\hat{R}_{\mathcal{S}}(w) + \lambda \|w\|_2^2\right) - \left(\hat{R}_{\mathcal{S}}(u) + \lambda \|u\|_2^2\right) \\
&= \left(\hat{R}_{\mathcal{S}^{(i)}}(w) + \lambda \|w\|_2^2\right) - \left(\hat{R}_{\mathcal{S}^{(i)}}(u) + \lambda \|u\|_2^2\right) \\
&\quad + \frac{\ell(w, z_i) - \ell(u, z_i)}{m} + \frac{\ell(u, z') - \ell(w, z')}{m} \\
&= \tilde{R}_{\mathcal{S}^{(i)}}(w) - \tilde{R}_{\mathcal{S}^{(i)}}(u) + \frac{\ell(w, z_i) - \ell(u, z_i)}{m} + \frac{\ell(u, z') - \ell(w, z')}{m}
\end{aligned}$$

Choosing $w = \mathfrak{A}\left(\mathcal{S}^{(i)}\right)$ and $u = \mathfrak{A}(\mathcal{S})$, and the fact that $\tilde{R}_{\mathcal{S}^{(i)}}\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right)\right) \leq \tilde{R}_{\mathcal{S}^{(i)}}(\mathfrak{A}(\mathcal{S}))$, it is

$$\tilde{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right)\right) - \tilde{R}_{\mathcal{S}}(\mathfrak{A}(\mathcal{S})) \leq \frac{\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell(\mathfrak{A}(\mathcal{S}), z_i)}{m} + \frac{\ell(\mathfrak{A}(\mathcal{S}), z') - \ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z'\right)}{m} \tag{4.5}$$

Note 35. Then (4.4) and (4.5) imply

$$\lambda \left\|\mathfrak{A}\left(\mathcal{S}^{(i)}\right) - \mathfrak{A}(\mathcal{S})\right\| \leq \frac{\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell(\mathfrak{A}(\mathcal{S}), z_i)}{m} + \frac{\ell(\mathfrak{A}(\mathcal{S}), z') - \ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z'\right)}{m} \tag{4.6}$$

Note 36. Now that we brought it in form (4.6), we can impose/use an additional assumption on the loss to bound it. In this example we use Lipstchitzness.

Assumption 37. *The loss function $\ell(\cdot, z)$ in (4.2) is convex and ρ-Lipschitz for any $z \in \mathcal{Z}$.*

Note 38. Given ρ-Lipschitzness in Assumption 37, it is

$$\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right) \leq \rho \left\|\mathfrak{A}\left(\mathcal{S}^{(i)}\right) - \mathfrak{A}\left(\mathcal{S}\right)\right\| \tag{4.7}$$

$$\ell\left(\mathfrak{A}\left(\mathcal{S}\right), z'\right) - \ell\left(\mathcal{S}^{(i)}, z'\right) \leq \rho \left\|\mathfrak{A}\left(\mathcal{S}^{(i)}\right) - \mathfrak{A}\left(\mathcal{S}\right)\right\| \tag{4.8}$$

and hence plugging 4.7 and (4.8) in (4.6) yields

$$\left\|\mathfrak{A}\left(\mathcal{S}^{(i)}\right) - \mathfrak{A}\left(\mathcal{S}\right)\right\| \leq 2\frac{\rho}{\lambda m} \tag{4.9}$$

Note 39. Plugging (4.9) in (4.7) yields

$$\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right) \leq 2\frac{\rho^2}{\lambda m}$$

Note 40. Using Theorem 19, we get an upper bound for the stability / over-fitting

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right) - \hat{R}_{\mathcal{D}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) = \mathrm{E}_{\substack{\mathcal{S}\sim g,\, z'\sim g \\ i\sim \mathrm{U}\{1,...,m\}}}\left(\ell\left(\mathfrak{A}\left(\mathcal{S}^{(i)}\right), z_i\right) - \ell\left(\mathfrak{A}\left(\mathcal{S}\right), z_i\right)\right) \leq 2\frac{\rho^2}{\lambda m}$$

Note 41. After this saga, the researcher could come to the conclusion that: A Ridge RLM learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with the loss function which is convex and ρ-Lipschitz, regularizer $J\left(\cdot;\lambda\right) = \lambda\left\|\cdot\right\|^2$, $\lambda > 0$, and learning rule trained against an iid sample $\mathcal{S} = \{z_i\}_{i=1}^m$ from g is on-averave-replace-one-stable with rate $\epsilon\left(m\right) = 2\frac{\rho^2}{\lambda m}$; i.e.

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right) - \hat{R}_{\mathcal{S}}\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq 2\frac{\rho^2}{\lambda m} \tag{4.10}$$

Note 42. From (4.10), we see that stability improves (and over-fitting decreases) as the shrinkage parameter λ increases.

4.3. **Bounding the Risk (2.3).**

Note 43. Given the bounds (4.3) and (4.10), the decomposition of the expected Risk in (2.3) yields that: A Ridge RLM learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with the loss function which is convex and ρ-Lipschitz, regularizer $J\left(\cdot;\lambda\right) = \lambda\left\|\cdot\right\|^2$, $\lambda > 0$, and learning rule trained against an iid sample $\mathcal{S} = \{z_i\}_{i=1}^m$ from g has Expected Risk bound

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \underbrace{R_g\left(w\right) + \lambda\left\|w\right\|_2^2}_{\text{(I)}} + \underbrace{2\frac{\rho^2}{\lambda m}}_{\text{(II)}}; \quad \forall w \in \mathcal{W} \tag{4.11}$$

Note 44. From 4.11, we see that there is a trade-off between Empirical Risk (I) and stability/overfitting (II) with regards the regularization parameter λ. It is desirable to use the optimal $\lambda > 0$ corresponding to the smallest bound in (4.11); it has to both fit the training data well (but perhaps not too well) and be very stable to different training data from the same g (but perhaps not too stable)!

Assumption 45. *Assume that the learning problem is additionally B-bounded by $B > 0$,; i.e.* $\mathcal{H} = \left\{w \in \mathbb{R}^d : \left\|w\right\|_2^2 \leq B\right\}$.

Note 46. If additionally the learning problem is B-bounded then the upper bound in (4.11) becomes

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \underbrace{\min_{w\in\mathcal{H}} R_g\left(w\right) + \lambda B}_{\text{(I)}} + \underbrace{2\frac{\rho^2}{\lambda m}}_{\text{(II)}} \tag{4.12}$$

Note 47. Furthermore, if we choose a shrinkage parameter $\lambda_m = \sqrt{\frac{2}{m}}\frac{\rho}{B}$ in (4.2) the upper bound in (4.11) becomes

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \min_{w\in\mathcal{H}} R_g\left(w\right) + \lambda_m B\sqrt{\frac{8}{m}} \tag{4.13}$$

4.4. **Deriving PAC guarantees.**

Note 48. In particular, if the size m of the training sample $\mathcal{S}$ is

$$m \geq \frac{\lambda_m^2 B^2 8}{\epsilon^2} = \frac{8\rho^2 B^2}{\epsilon^2}$$

for some $\epsilon > 0$ then for every distribution g, the upper bound in (4.11) becomes

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \min_{w\in\mathcal{H}} R_g\left(w\right) + \epsilon \tag{4.14}$$

and hence we can have a PAC guarantee that is summarized in the following.

Summary 49. Let $(\mathcal{H}, \mathcal{Z}, \ell)$ be a learning problem convex-Lipschitz-bounded with parameters ρ and B, and let m be the training data size. The associated Ridge Regularized Loss Minimization rule with regularization function $\lambda_m = \sqrt{\frac{2}{m}}\frac{\rho}{B}$ satisfies

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \min_{w\in\mathcal{H}} R_g\left(w\right) + \lambda_m B\sqrt{\frac{8}{m}}$$

Moreover, if $m \geq \frac{8\rho^2 B^2}{\epsilon^2}$, $\epsilon > 0$ then for every distribution g we can get a PAC -guarantee

$$\mathrm{E}_{\mathcal{S}\sim g}\left(R_g\left(\mathfrak{A}\left(\mathcal{S}\right)\right)\right) \leq \min_{w\in\mathcal{H}} R_g\left(w\right) + \epsilon$$

Appendix A. Recall strong convex functions from Handout 2.

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

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

- The function $f\left(w\right) = \lambda\left\|w\right\|_2^2$ is 2λ-strongly convex
- If $f$is λ-strongly convex and g is convex then $f+g$ is λ-strongly convex
- If $f$is λ-strongly convex and u is a minimizer of f then for any w

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

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

Handout 4: Gradient descent

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Aim. To introduce gradient descent, its motivation, description, practical tricks, analysis in the convex scenario, and implementation.

Reading list & references:

(1) Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
- Ch. 14.1 Gradient Descent

1. Motivations

Problem 1. Consider a learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$. Learning may involve the computation of the minimizer $h^* \in \mathcal{H}$, where $\mathcal{H}$ is a class of hypotheses, of the empirical risk function (ERF) $\hat{R}(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h, z_i)$ given a finite sample $\{z_i; i = 1, ..., n\}$ generated from the data generating model $g(\cdot)$ and using loss $\ell(\cdot)$; that is

$$h^* = \arg\min_{h\in\mathcal{H}} \left(\hat{R}(h)\right) = \arg\min_{h\in\mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^{n} \ell(h, z_i)\right) \tag{1.1}$$

If analytical minimization of (1.1) is impossible or impractical, numerical procedures can be applied; eg Gradient Descent (GD) algorithms. Such approaches introduce numerical errors in the solution.

2. Description

Problem 2. For the sake of notation simplicity and generalization, we will present Gradient Descent (GD) in the following minimization problem

$$w^* = \arg\min_{w\in\mathcal{H}} (f(w)) \tag{2.1}$$

where here $f : \mathbb{R}^d \to \mathbb{R}$, and $w \in \mathcal{H} \subseteq \mathbb{R}^d$; $f(\cdot)$ is the function to be minimized, e.g., $f(\cdot)$ can be an empirical risk function $\hat{R}(\cdot)$.

Assumption 3. *Assume (for now) that $f : \mathbb{R}^d \to \mathbb{R}$ is a differentiable function.*

Algorithm 4. *Gradient Descent (GD) algorithm with learning rate $\eta_t > 0$ for the solution of the minimization problem (2.1)*

For $t = 1, 2, 3, ...$ iterate:

(1) *compute*

$$w^{(t+1)} = w^{(t)} - \eta_t \nabla f\left(w^{(t)}\right) \tag{2.2}$$

(2) *terminate if a termination criterion is satisfied, e.g.*

$$\textit{If } t \geq T_{\max} \textit{ then STOP}$$

Note 5. Recall that the gradient of $f : \mathbb{R}^d \to \mathbb{R}$ at w is

$$\nabla f(w) = \left(\frac{\partial}{\partial x_1} f(x), \ldots, \frac{\partial}{\partial x_d} f(x)\right)^\top \Bigg|_{x=w}.$$

Note 6. (Intuition) GD produces a chain $\left\{w^{(t)}\right\}$ that drifts towards a minimum w^*. It evolves directed towards the opposite direction than that of the gradient $\nabla f(\cdot)$ and at a rate controlled by the learning rate η_t.

Note 7. (More intuition) Consider the (1st order) Taylor polynomial for the approximation of $f(w)$ in a small area around u (i.e. $\|v - u\| = \text{small}$)

$$f(u) \approx P(u) = f(w) + \langle u - w, \nabla f(w) \rangle$$

Assuming convexity for f, it is

$$f(u) \geq \underbrace{f(w) + \langle u - w, \nabla f(w) \rangle}_{=P(u;w)} \tag{2.3}$$

meaning that P lower bounds f. Hence we could design an updating mechanism producing $w^{(t+1)}$ which is nearby $w^{(t)}$ (small steps) and which minimize the linear approximation $P(w)$ of $f(w)$ at $w^{(t)}$

$$P\left(w; w^{(t)}\right) = f\left(w^{(t)}\right) + \langle w - w^{(t)}, \nabla f\left(w^{(t)}\right) \rangle. \tag{2.4}$$

while hoping that this mechanism would push the produced chain $\left\{w^{(t)}\right\}$ towards the minimum because of (2.3). Hence we could recursively minimize the linear approximation (2.4) and the distance between the current state $w^{(t)}$ and the next w value to produce $w^{(t+1)}$; namely

$$\begin{aligned} w^{(t+1)} &= \arg\min_{\forall w} \left(\frac{1}{2}\left\|w - w^{(t)}\right\|^2 + \eta P\left(w; w^{(t)}\right)\right) \\ &= \arg\min_{\forall w} \left(\frac{1}{2}\left\|w - w^{(t)}\right\|^2 + \eta\left(f\left(w^{(t)}\right) + \langle w - w^{(t)}, \nabla f\left(w^{(t+1)}\right)\rangle\right)\right) \\ &= w^{(t)} - \eta \nabla f\left(w^{(t)}\right) \end{aligned} \tag{2.5}$$

where parameter $\eta > 0$ controls the trade off in (2.5).

Note 8. Given T iterations of GD algorithm, the output of GD can be (but not a exclusively),

(1) the average (after discarding the first few iterations of $w^{(t)}$ for stability reasons)

$$w_{\text{GD}}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)} \tag{2.6}$$

(2) or the best value discovered

$$w_{\text{GD}}^{(T)} = \arg\min_{\forall w_t} \left(f\left(w^{(t)} \right) \right)$$

(3) or the last value discovered

$$w_{\text{GD}}^{(T)} = w^{(T)}$$

Note 9. GD output (e.g. in Note 8) converges to a local minimum, $w_{\text{GD}}^{(T)} \to w_*$ (in some sense), under different sets of regularity conditions (some are weaker other stronger). Section 4 has a brief analysis.

Note 10. The parameter η_t is called learning rate (or step size, gain). It determines the size of the steps GD takes to reach a (local) minimum. $\{\eta_t\}$ is a non-negative sequence and it is chosen by the practitioner. In principle, regularity conditions (Note 9) often imply restrictions on the decay of $\{\eta_t\}$ which guide the practitioner to parametrize it properly. Some popular choices of learning rate η_t are:

(1) constant; $\eta_t = \eta$, for where $\eta > 0$ is a small value. The rationale is that GD chain $\{w_t\}$ performs constant small steps towards the (local) minimum w_* and then oscillate around it.

(2) decreasing and converging to zero; $\eta_t \searrow$ with $\lim_{t\to\infty} \eta_t = 0$. E.g. $\eta_t = \left(\frac{C}{t}\right)^{\varsigma}$ where $\varsigma \in [0.5, 1]$ and $C > 0$. The rationale is that GD algorithm starts by performing larger steps (controlled by C) at the beginning to explore the area for discovering possible minima. Also it reduces the size of those steps with the iterations (controled by ς) such that eventually when the chain $\{w_t\}$ is close to a possible minimum w_* value to converge and do not overshoot.

(3) decreasing and converging to a tiny value τ_*; $\eta_t \searrow$ with $\lim_{t\to\infty} \eta_t = \tau_*$ E.g. $\eta_t = \left(\frac{C}{t}\right)^{\varsigma} + \tau_*$ with $\varsigma \in (0.5, 1]$, $C > 0$, and $\tau_* \approx 0$. Same as previously, but the algorithm aims at oscillating around the detected local minimum.

(4) constant until an iteration T_0 and then decreasing; Eg $\eta_t = \left(\frac{C}{\max(t, T_0)}\right)^{\varsigma}$ with $\varsigma \in [0.5, 1]$ and $C > 0$, and $T_0 < T$. The rationale is that at the first stage of the iterations (when $t \le T_0$) the algorithm may need a constant large steps for a significant number of iterations T_0 in order to explore the domain; and hence in order for the chain $\{w_t\}$ to reach the area around the (local) minimum w_*. In the second stage, hoping that the chain $\{w_t\}$ may be in close proximity to the (local) minimum w_* the algorithm progressively performs smaller steps to converge towards the minimum w_*. The first stage ($t \le T_0$) is called burn-in; the values $\{w_t\}$ produced during the burn-in ($t \le T_0$) are are often discarded/ignored from the output of the GD algorithm.

- Parameters $C, \varsigma, \tau_*, T_0$ may be chosen based on pilot runs against a small fraction of the training data set.

Note 11. There are several practical termination criteria that can be used in GD Algorithm 4(step 2). They aim to terminate the recursion in practice. Some popular termination criteria are

(1) terminate when the gradient is sufficiently close to zero; i.e. if $\left\|\nabla f\left(w^{(t)}\right)\right\| \leq \epsilon$ for some pre-specified tiny $\epsilon > 0$ then STOP
(2) terminate when the chain $w^{(t)}$ does not change; i.e. if $\left\|w^{(t+1)} - w^{(t)}\right\| \leq \epsilon \left\|w^{(t)}\right\|$ for some pre-specified tiny $\epsilon > 0$ then STOP
(3) terminate when a pre-specified number of iterations T is performed; i.e. if $t \geq T$ then STOP

Here (1) may be deceive if the chain is in a flat area, (2) may be deceived if the learning rate become too small, (3) is obviously a last resort.

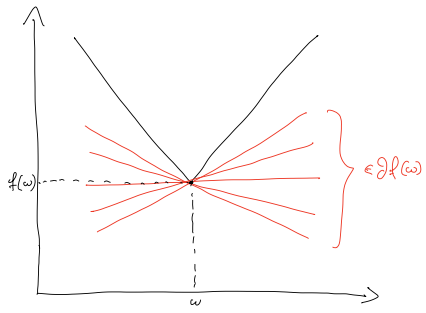
3. GD for non-differentiable functions (using sub-gradients)

Note 12. In several learning problems the function to be minimized is not differentiable. GD can be extended to address such problems with the use of subgradients.

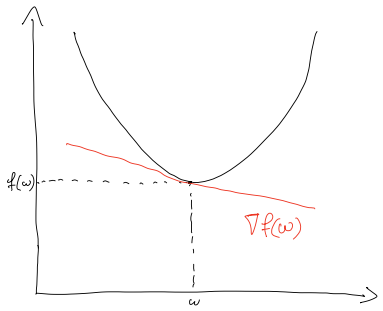
Definition 13. Vector v is called subgradient of a function $f : S \to \mathbb{R}$ at $w \in S$ if

$$\forall u \in S, \quad f(u) \geq f(w) + \langle u - w, v \rangle \tag{3.1}$$

Note 14. Essentially there may be more than one subgradients of the function at a specific point. As seen by (3.1), subgradients are the slopes of all the lines passing through the point $(w, f(w))$ and been under the function $f(\cdot)$.



(A) subgradients satisfying (3.1) in the non-differentiable case



(B) gradient satisfying the equality in (3.1) in the differentiable case

Definition 15. The set of subgradients of function $f : S \to \mathbb{R}$ at $w \in S$ is denoted by $\partial f(w)$.

Algorithm 16. *The Gradient Descent algorithm using subgradients in non-differentiable cases, results by replacing the gradient $\nabla f\left(w^{(t)}\right)$ in (2.2) with any of subgradient v_t from the set of subgradients $\partial f\left(w^{(t)}\right)$ at $w^{(t)}$; namely (2.2) is replaced by*

$$w^{(t+1)} = w^{(t)} - \eta_t v_t; \quad \textit{where } v_t \in \partial f\left(w^{(t)}\right) \tag{3.2}$$

3.1. **Construction of subgradient.**

Note 17. We discuss how to construct subgradients in practice.

Fact 18. *Some properties of subgradient sets that help for their construction*

(1) *If function $f : S \to \mathbb{R}$ is differentiable at w then the only subgradient of f at w is the gradient $\nabla f(w)$, and (3.1) is equality; i.e. $\partial f(w) = \{\nabla f(w)\}$.*
(2) *for constants α, β and convex function $f(\cdot)$, it is*

$$\partial(\alpha f(w) + \beta) = \alpha(\partial f(w)) = \{\alpha v : v \in \partial f(w),\}$$

(3) *for convex functions $f(\cdot)$ and $g(\cdot)$, it is*

$$\partial(f(w) + g(w)) = \partial f(w) + \partial g(w) = \{v + u : v \in \partial f(w),\ and\, u \in \partial g(w)\}$$

Example 19. Consider the function $f : \mathbb{R} \to \mathbb{R}_+$ with $f(w) = |w| = \begin{cases} w & w \geq 0 \\ -w & w < 0 \end{cases}$. Find the set of subgradients $\partial f(w)$ for each $w \in \mathbb{R}$.

Solution. Using Fact 18, it is $\partial f(w) = 1$ for $w > 0$ and $\partial f(w) = -1$ for $w < 0$ as f is differentiable for $x \neq 0$. At $x = 0$, f is not differentiable; hence from condition (3.1) it is

$$\forall u \in \mathbb{R},\ \ |u| \geq |0| + (u - 0)\, v$$

which is satisfied for $v \in [-1, 1]$. Hence,

$$\partial f(w) = \begin{cases} \{-1\} & , w < 0 \\ [-1, 1] & , w = 0 \\ \{1\} & , w > 0 \end{cases}$$

4. Analysis of Gradient descent (Algorithm 4)

Note 20. Recall we address the minimization Problem 2 under Assumptions 21.

Assumption 21. *For the sake of the analysis of the GD, let us consider:*

(1) *The function $f(\cdot)$ is convex and Lipschitz*
(2) *GD has a constant learning rate $\eta_t = \eta$,*
(3) *GD output $w_{GD}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)}$*

No need to memorize

Lemma 22. *Let $\{v_t; t = 1, ..., T\}$ be a sequence of vectors. Any algorithm with $w^{(1)} = 0$ and $w^{(t+1)} = w^{(t)} - \eta v_t$ for $t = 1, ..., T$ satisfies*

$$\sum_{t=1}^{T} \langle w^{(t)} - w^*, v_t \rangle \leq \frac{\|w^*\|^2}{2\eta} + \frac{\eta}{2}\sum_{t=1}^{T} \|v_t\|^2 \tag{4.1}$$

Proof. Omitted; see the Exercise 12 in the Exercise sheet 1. □

Note 23. To find an upper bound of the GD error, we try to bound the error $f\left(w_{\mathrm{GD}}^{(T)}\right)-f\left(w^{*}\right)$ with purpose to use Lemma 22.

Proposition 24. *Consider the minimization problem (2.1). Given Assumptions 21, the error can be bounded as*

$$f\left(w_{GD}^{(T)}\right)-f\left(w^{*}\right)\leq\frac{\left\|w^{*}\right\|^{2}}{2\eta T}+\frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T}\left\|v_{t}\right\|^{2} \tag{4.2}$$

where $v_t \in \partial f\left(w^{(t)}\right)$. *If* $f(\cdot)$ *is differentiable then* $v_t = \nabla f\left(w^{(t)}\right)$

Proof. It is[1]

$$\begin{aligned}
f\left(w_{\mathrm{GD}}^{(T)}\right)-f\left(w^{*}\right) =& f\left(\frac{1}{T}\sum_{t=1}^{T}w_{t}\right)-f\left(w^{*}\right)\\
\leq& \frac{1}{T}\sum_{t=1}^{T}\left(f\left(w_{t}\right)-f\left(w^{*}\right)\right) && \text{(by Jensen's inequality)} \qquad (4.3)\\
\leq& \frac{1}{T}\sum_{t=1}^{T}\langle w^{(t)}-w^{*},v_{t}\rangle && \text{(by convexity of } f(\cdot)) \\
\leq& \frac{\left\|w^{*}\right\|^{2}}{2\eta T}+\frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T}\left\|v_{t}\right\|^{2} && \text{(by roceeding Lemma)} \qquad (4.4)
\end{aligned}$$

□

Note 25. Proposition 24 shows that it is important to bound the (sub-)gradient in (4.2) in a meaningful manner. Lemma 26 shows that if we assume Lipschitzness as well, the (sub-)gradient has the so-called self-bounded behavior.

Lemma 26. [2] $f: S \to \mathbb{R}$ *is* ρ*-Lipschitz over an open convex set* S *if and only if for all* $w \in S$ *and* $v \in \partial f(w)$ *it is* $\|v\| \leq \rho$.

Proof. $\Longrightarrow$ Let $f: S \to \mathbb{R}$ be ρ-Lipschitz over convex set S, $w \in S$ and $v \in \partial f(w)$.

- Since S is open we get that there exist $\epsilon > 0$ such as $u := w + \epsilon\frac{v}{\|v\|}$ where $u \in S$. So $\langle u-w, v\rangle = \epsilon\|v\|$ and $\|u-w\| = \epsilon$.
- From the subgradient definition we get

$$f(u) - f(w) \geq \langle u-w, v\rangle = \epsilon\|v\|$$

- From the Lipschitzness of $f(\cdot)$ we get

$$f(u) - f(w) \leq \rho\|u-w\| = \rho\epsilon$$

[1] Jensen's inequality for convex $f(.)$ is $f(\mathrm{E}(x)) \leq \mathrm{E}(f(x))$

[2] If this was a Homework there would be a Hint:

- If S is open there exist $\epsilon > 0$ such as $u = w + \epsilon\frac{v}{\|v\|}$ such as $u \in S$

Therefore $\|v\| \leq \rho$.

For $\Longleftarrow$ see Exercise 4 in the Exercise sheet. □

Note 27. The following summaries Proposition 24 and Lemma 26 with respect to the GD algorithm satisfying Assumption 21.

Proposition 28. *Let $f(\cdot)$ be a convex and ρ-Lipschitz function. If we run GD algorithm of f with learning rate $\eta > 0$ for T steps the output $w_{\mathrm{GD}}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)}$* satisfies

$$f\left(w_{\mathrm{GD}}^{(T)}\right) - f\left(w^*\right) \leq \frac{\|w^*\|^2}{2\eta T} + \frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T}\left\|\nabla f\left(w^{(t)}\right)\right\|^2$$

where $\|\nabla f(\cdot)\| \leq \rho$.

Solution. Straightforward from Lemma 22 and Proposition 24.

Note 29. The following shows that a given learning rate depending on the iteration t, we can reduce the upper bound of the error as well as find the number of required iterations to achieve convergence.

Proposition 30. *(Cont Prop. 28) Let $f(\cdot)$ be a convex and ρ-Lipschitz function, and let $\mathcal{H} = \{w \in \mathbb{R} : \|w\| \leq B\}$. Assume we run GD algorithm of $f(\cdot)$ with learning rate $\eta_t = \sqrt{\frac{B^2}{\rho^2 T}}$ for T steps, and output $w_{\mathrm{GD}}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)}$. Then*

(1) *upper bound on the sub-optimality is*

$$f\left(w_{\mathrm{GD}}^{(T)}\right) - f\left(w^*\right) \leq \frac{B\rho}{\sqrt{T}} \tag{4.5}$$

(2) *a given level off accuracy ε such that $f\left(w_{GD}^{(T)}\right) - f\left(w^*\right) \leq \varepsilon$ can be achieved after T iterations*

$$T \geq \frac{B^2\rho^2}{\varepsilon^2}.$$

Proof. Part 1 is a simple substitution from Proposition 28, and part 2 is implied from part 1. □

Note 31. The result on Proposition 30 heavily relies on setting suitable values for B and ρ which is rather a difficult task to be done in very complicated learning problems (e.g., learning a neural network).

Note 32. The above results from the analysis of the GD also hold for the GD with subgradients; just replace $\nabla f(\cdot)$ with any v_t such that $v_t \in \partial f(\cdot)$.

5. Examples [3]

Example 33. Consider the simple Normal linear regression problem where the dataset $\{z_i = (y_i, x_i)\}_{i=1}^n \in \mathcal{D}$ is generated from a Normal data generating model

$$\begin{pmatrix} y_i \\ x_i \end{pmatrix} \overset{\text{iid}}{\sim} \mathrm{N}\left(\begin{pmatrix} \mu_y \\ \mu_x \end{pmatrix}, \begin{bmatrix} \sigma_y^2 & \rho\sqrt{\sigma_y^2\sigma_x^2} \\ \rho\sqrt{\sigma_y^2\sigma_x^2} & \sigma_x^2 \end{bmatrix}\right) \tag{5.1}$$

[3] Code is available in `https://github.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2024/tree/main/Lecture_handouts/code/04.Gradient_descent/example_1.R`

for $i = 1, ..., n$. Consider a hypothesis space $\mathcal{H}$ of linear functions $h : \mathbb{R}^2 \to \mathbb{R}$ with $h(w) = w_1 + w_2 x$. The exact solution (which we pretend we do not know) is given as

$$\begin{pmatrix} w_1^* \\ w_2^* \end{pmatrix} = \begin{pmatrix} \mu_y - \rho \frac{\sigma_y}{\sigma_x} \mu_x \\ \rho \frac{\sigma_y}{\sigma_x} \end{pmatrix}. \tag{5.2}$$

To learn the optimal $w^* = (w_1^*, w_2^*)^\top$, we consider a loss $\ell\left(w, z_i = (x_i, y_i)^\top\right) = (y_i - [w_1 + w_2 x_i])^2$, which leads to the minimization problem

$$w^* = \arg\min_w \left(\hat{R}_{\mathcal{D}}(w)\right) = \arg\min_w \left(\frac{1}{n} \sum_{i=1}^{n} (y_i - w_1 - w_2 x_i)^2\right)$$

The GD Algorithm 4 with learning rate η is

For $t = 1, 2, 3, ...$ iterate:

(1) compute

$$w^{(t+1)} = w^{(t)} - \eta v_t, \qquad \text{where } v_t = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \bar{x} - 2\bar{y} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \overline{x^2} - 2y^\top x \end{pmatrix} \tag{5.3}$$

(2) terminate if a termination criterion is satisfied, e.g.

$$\text{If } t \geq T \text{ then STOP}$$

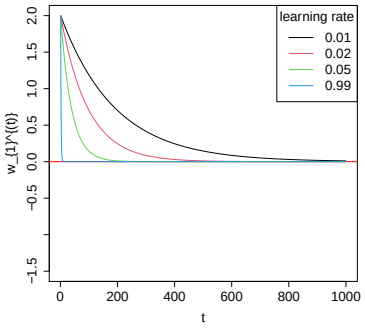
This is because $\hat{R}_{\mathcal{D}}(w)$ is differentiable in $\mathbb{R}^2$ so $\partial \hat{R}_{\mathcal{D}}(w) = \left\{\nabla \hat{R}_{\mathcal{D}}(w)\right\}$ and because

$$\nabla \hat{R}_{\mathcal{D}}(w) = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}w_1} \hat{R}_{\mathcal{D}}(w) \\ \frac{\mathrm{d}}{\mathrm{d}w_2} \hat{R}_{\mathcal{D}}(w) \end{pmatrix} = ... = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \bar{x} - 2\bar{y} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \overline{x^2} - 2y^\top x \end{pmatrix}$$

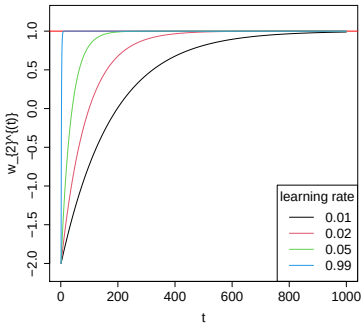
Consider data size $n = 100$, and parameters $\rho = 0.2$, $\sigma_y^2 = 1$ and $\sigma_x^2 = 1$. Then the real value (5.2) that I need to learn equals to $w^* = (0, 1)^\top$. Consider a GD seed $w_0 = (2, -2)$, and total number of iterations $T = 1000$.

Figures 5.1a, 5.1b, and 5.1c present trace plots of the chain $\left\{\left(w^{(t)}\right)\right\}$ and error $\hat{R}_{\mathcal{D}}\left(w^{(t)}\right) - \hat{R}_{\mathcal{D}}(w^*)$ produced by running GD for $T = 1000$ total iterations and for different (each time) constant learning rates $\eta \in \{0.01, 0.02, 0.05, 0.99\}$. We observe that the larger learning rates under consideration were able to converge faster to the minimum w^*. This is because they perform larger steps and can learn faster -this is not a panacea.

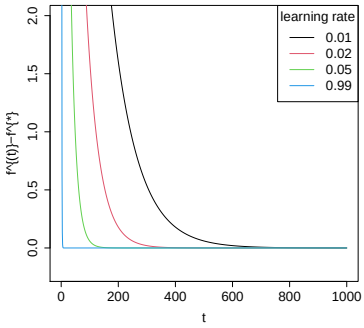
Figures 5.1d, 5.1e, and 5.1f present trace plots of the chain $\left\{\left(w^{(t)}\right)\right\}$, and of the error $\hat{R}_{\mathcal{D}}\left(w^{(t)}\right) - \hat{R}_{\mathcal{D}}(w^*)$ produced by running GD for $T = 1000$ total iterations and for learning rate $\eta = 1.0$ (previously considered) and a very big learning rate $\eta = 3.0$. We observe that the very big learning rate $\eta = 3.0$ presents slower convergence to the minimum w^*. This is because it creates unreasonably big steps in (2.2) that the produced chain overshoots the global minimum; see the cartoon in Figures 5.1g and 5.1h.



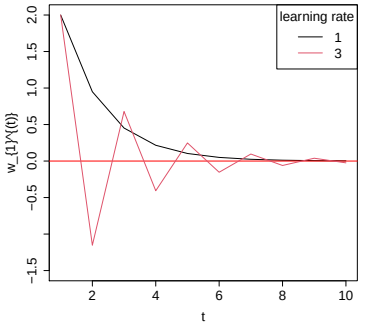
(A) $\left\{\left(w_1^{(t)}\right)\right\}$



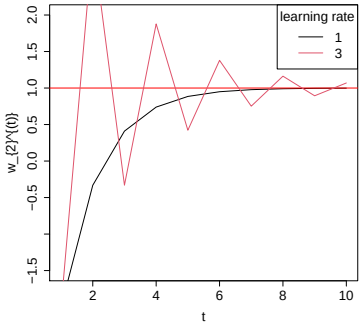
(B) $\left\{\left(w_2^{(t)}\right)\right\}$



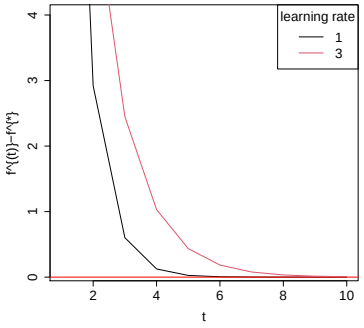
(C) $\hat{R}_{\mathcal{D}}\left(w^{(t)}\right) - \hat{R}_{\mathcal{D}}\left(w^*\right)$



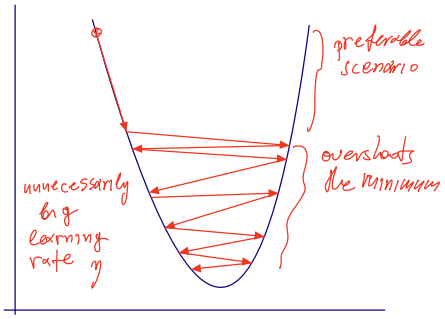
(D) $\left\{\left(w_1^{(t)}\right)\right\}$



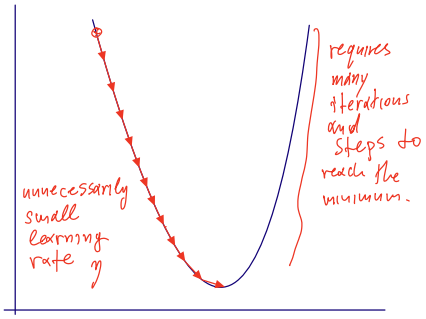
(E) $\left\{\left(w_2^{(t)}\right)\right\}$



(F) $\hat{R}_{\mathcal{D}}\left(w^{(t)}\right) - \hat{R}_{\mathcal{D}}\left(w^*\right)$



(G) Unnecessarily large learning rate



(H) Unnecessarily small learning rate

FIGURE 5.1

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

Handout 5: Stochastic gradient descent

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Aim. To introduce the stochastic gradient descent (motivation, description, practical tricks, analysis in the convex scenario, and implementation).

Reading list & references:

(1) Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
- Ch. 14.3 Stochastic Gradient Descent (SGD), 14.5 Variants, 14.5 Learning with SGD

(2) Bottou, L. (2012). Stochastic gradient descent tricks. In Neural networks: Tricks of the trade (pp. 421-436). Springer, Berlin, Heidelberg.

(3) Johnson, Rie, and Tong Zhang. "Accelerating stochastic gradient descent using predictive variance reduction." Advances in neural information processing systems 26 (2013).

(4) Duchi, John, Elad Hazan, and Yoram Singer. "Adaptive subgradient methods for online learning and stochastic optimization." Journal of machine learning research 12, no. 7 (2011).

Code of the Examples can be found in `https://github.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2024/tree/main/Lecture_handouts/code/05.Stochastic_gradient_descent`

1. Motivations for stochastic gradient descent

Problem 1. Consider a learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$. Learning may involve the computation of the minimizer $w^* \in \mathcal{H}$, where $\mathcal{H}$ is a class of hypotheses, of the risk function (RF) $R(w) = \mathrm{E}_{z\sim g}(\ell(w,z))$ given an unknown data generating model $g(\cdot)$ and using a known tractable loss $\ell(\cdot,\cdot)$; that is

$$w^* = \arg\min_{\forall w\in\mathcal{H}} (R_g(w)) = \arg\min_{\forall w\in\mathcal{H}} (\mathrm{E}_{z\sim g}(\ell(w,z))) \tag{1.1}$$

Note 2. Gradient descent (GD) cannot be directly utilized to address Problem 1 (i.e., minimize the Risk function) because g is unknown, and because (1.1) involves an integral which may be computationally intractable. Instead it aims to minimize the ERF $\hat{R}(w) = \frac{1}{n}\sum_{i=1}^{n} \ell(w, z_i)$ which ideally is used as a proxy when data size n is big (big-data).

Note 3. The implementation of GD may be computationally impractical even in problems where we need to minimize an ERF $\hat{R}_n(w)$ if we have big data ($n \approx$big). This is because GD requires the recursive computation of the exact gradient $\nabla\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n} \nabla\ell(w, z_i)$ using all the data $\{z_i\}$ at each iteration. That may be too slow.

Note 4. Stochastic gradient descent (SGD) aims at solving (1.1), and overcoming the issues in Notes 2 & 3 by using an unbiased estimator of the actual gradient (or some sub-gradient) based on a sample (a single example or a set of examples) properly drawn from g.

2. Stochastic gradient descent

Problem 5. For the sake of notation simplicity and generalization, we present Stochastic Gradient Descent (SGD) in the following minimization problem

$$w^* = \arg\min_{w\in\mathcal{H}} \left(f\left(w\right)\right) \tag{2.1}$$

where here $f : \mathbb{R}^d \to \mathbb{R}$, and $w \in \mathcal{H} \subseteq \mathbb{R}^d$; $f\left(\cdot\right)$ is the unknown function to be minimized, e.g., $f\left(\cdot\right)$ can be the risk function $R_g\left(w\right) = \mathrm{E}_{z\sim g}\left(\ell\left(w,z\right)\right)$.

Algorithm 6. *Stochastic Gradient Descent (SGD) with learning rate $\eta_t > 0$ for the solution of the minimization problem 5*

For $t = 1, 2, 3, ...$ iterate:

(1) *compute*

$$w^{(t+1)} = w^{(t)} - \eta_t v_t, \tag{2.2}$$

where v_t is a random vector such that $E\left(v_t|w^{(t)}\right) \in \partial f\left(w^{(t)}\right)$

(2) *terminate if a termination criterion is satisfied, e.g.*

$$\textit{If } t \geq T_{\max} \textit{ then STOP}$$

Note 7. If f is differentiable at $w^{(t)}$, it is $\partial f\left(w^{(t)}\right) = \left\{\nabla f\left(w^{(t)}\right)\right\}$. Hence v_t is such as $\mathrm{E}\left(v_t|w^{(t)}\right) = \nabla f\left(w^{(t)}\right)$ in Algorithm 6 step 1.

Note 8. Assume f is differentiable (for simplicity). To compare SGD with GD, we can re-write (2.2) in the SGD Algorithm 6 as

$$w^{(t+1)} = w^{(t)} - \eta_t \left[\nabla f\left(w^{(t)}\right) + \xi_t\right], \tag{2.3}$$

where

$$\xi_t := v_t - \nabla f\left(w^{(t)}\right)$$

represents the (observed) noise introduced in (2.2) by using a random realization of the exact gradient.

Note 9. Given T SGD algorithm iterations, the output of SGD can be (but not a exclusively)

(1) the average (after discarding the first few iterations of $w^{(t)}$ for stability reasons)

$$w_{\mathrm{SGD}}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)} \tag{2.4}$$

(2) or the best value discovered

$$w_{\mathrm{SGD}}^{(T)} = \arg\min_{\{w_t\}} \left(f\left(w^{(t)}\right)\right)$$

(3) or the last value discovered

$$w_{\mathrm{SGD}}^{(T)} = w^{(T)}$$

Note 10. SGD output converges to a local minimum, $w_{\text{SGD}}^{(T)} \to w_*$ (in some sense), under different sets of regularity conditions –Section 3 has a brief analysis. To achieve this, Conditions 11 on the learning rate are rather inevitable and should be satisfied.

Condition 11. Regarding the learning rate (or gain) $\{\eta_t\}$ should satisfy conditions

(1) $\eta_t \geq 0$,
(2) $\sum_{t=1}^{\infty} \eta_t = \infty$
(3) $\sum_{t=1}^{\infty} \eta_t^2 < \infty$

Note 12. The popular learning rates $\{\eta_t\}$ in Note 8 in Handout 4 "Gradient descent" satisfy Condition 11 and hence can be used in SGD too. Once parameterized, η_t can be tuned based on pilot runs using a reasonably small fraction of the training data set.

Note 13. (Intuition on Condition 11). Assume that v_t is bounded. Condition 11(3) aims at reducing the effect of the randomness in v_t (introduced noise ξ_t) because it implies $\eta_t \searrow 0$ as $t \to \infty$; if this was not the case then

$$w^{(t+1)} - w^{(t)} = -\eta_t v_t \to 0$$

may not be satisfied and the chain $\left\{w^{(t)}\right\}$ may not converge. Condition 11(2) prevents η_t from reducing too fast and allows the generated chain $\left\{w^{(t)}\right\}$ to be able to converge. E.g., after t iterations

$$\begin{aligned}\left\|w^{(t)} - w^*\right\| &= \left\|w^{(t)} \pm w^{(0)} - w^*\right\| \geq \left\|w^{(0)} - w^*\right\| - \left\|w^{(t)} - w^{(0)}\right\| \\ &\geq \left\|w^{(0)} - w^*\right\| - \sum_{t=0}^{\infty} \left\|w^{(t+1)} - w^{(t)}\right\| = \left\|w^{(0)} - w^*\right\| - \sum_{t=0}^{T-1} \|\eta_t v_t\|\end{aligned}$$

However if it was $\sum_{t=1}^{\infty} \eta_t < \infty$ it would be $\sum_{t=0}^{\infty} \|\eta_t v_t\| < \infty$ and hence $w^{(t)}$ would never converge to w^* if the seed $w^{(0)}$ is far enough from w^*.

3. Analysis of SGD (Algorithm 6)

Note 14. Recall that the stochasticity of SGD comes from the stochastic sub-gradients $\{v_t\}$ in (2.2); hence the expectations below are under these random vectors' distributions.

Proposition 15. *Let $f(\cdot)$ be a convex function. If we run SGD algorithm of f with learning rate $\eta_t > 0$ for T steps, the output $w_{\text{GD}}^{(T)} = \frac{1}{T}\sum_{t=1}^{T} w^{(t)}$* satisfies

$$\mathrm{E}\left(f\left(w_{\text{SGD}}^{(T)}\right)\right) - f(w^*) \leq \frac{\|w^*\|^2}{2\eta T} + \frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T} \mathrm{E}\|v_t\|^2 \tag{3.1}$$

Proof. Let $v_{1:t} = (v_1, ..., v_t)$. By Jensens' inequality (or see 4.3 in Handout 4)

$$\mathrm{E}\left(f\left(w_{\text{SGD}}^{(T)}\right) - f(w^*)\right) \leq \mathrm{E}\left(\frac{1}{T}\sum_{t=1}^{T}\left(f\left(w^{(t)}\right) - f(w^*)\right)\right) = \frac{1}{T}\sum_{t=1}^{T}\mathrm{E}\left(f\left(w^{(t)}\right) - f(w^*)\right) \tag{3.2}$$

I will try to use Lemma 22 from Handout 4, hence I need to show

$$\mathrm{E}\left(f\left(w^{(t)}\right) - f(w^*)\right) \leq \mathrm{E}\left(\langle w^{(t)} - w^*, v_t\rangle\right) \tag{3.3}$$

where the expectation is under $v_{1:T}$. It is

$$\begin{aligned}\mathrm{E}_{v_{1:T}}\left(\langle w^{(t)}-w^{*},v_{t}\rangle\right) =&\mathrm{E}_{v_{1:t}}\left(\langle w^{(t)}-w^{*},v_{t}\rangle\right)\\ =&\mathrm{E}_{v_{1:t-1}}\left(\mathrm{E}_{v_{1:t}}\left(\langle w^{(t)}-w^{*},v_{t}\rangle|v_{1:t-1}\right)\right) \quad (\text{ law of total expectation })\end{aligned}$$

But $w^{(t)}$ is fully determined by $v_{1:t-1}$, (see (2.2)) so

$$\mathrm{E}_{v_{1:t-1}}\left(\mathrm{E}_{v_{1:t}}\left(\langle w^{(t)}-w^{*},v_{t}\rangle|v_{1:t-1}\right)\right) =\mathrm{E}_{v_{1:t-1}}\left(\langle w^{(t)}-w^{*},\mathrm{E}_{v_{1:t}}\left(v_{t}|v_{1:t-1}\right)\rangle\right)$$

As $w^{(t)}$ is fully determined by $v_{1:t-1}$ then $\mathrm{E}_{v_{1:t}}\left(v_{t}|v_{1:t-1}\right)=\mathrm{E}_{v_{1:t}}\left(v_{t}|w^{(t)}\right)\in\partial f\left(w^{(t)}\right)$, hence $\mathrm{E}_{v_{1:t}}\left(v_{t}|v_{1:t-1}\right)$ is a sub-gradient. By sub-gradient definition

$$\begin{aligned}\mathrm{E}_{v_{1:t-1}}\left(\langle w^{(t)}-w^{*},\mathrm{E}_{v_{1:t}}\left(v_{t}|v_{1:t-1}\right)\rangle\right) \geq&\mathrm{E}_{v_{1:t-1}}\left(f\left(w^{(t)}\right)-f\left(w^{*}\right)\right)\\ =&\mathrm{E}_{v_{1:T}}\left(f\left(w^{(t)}\right)-f\left(w^{*}\right)\right)\end{aligned} \tag{3.4}$$

Hence combining (3.4), (3.3), and (3.2)

$$\mathrm{E}\left(f\left(w_{\mathrm{SGD}}^{(T)}\right)-f\left(w^{*}\right)\right)\leq\frac{1}{T}\sum_{t=1}^{T}\mathrm{E}\left(\langle w^{(t)}-w^{*},v_{t}\rangle\right)$$

Then Lemma 22 in Handout 4 "Gradient descent" implies

$$\mathrm{E}\left(f\left(w_{\mathrm{SGD}}^{(T)}\right)-f\left(w^{*}\right)\right)\leq\mathrm{E}\left(\frac{1}{T}\frac{\left\|w^{*}\right\|^{2}}{2\eta}+\frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T}\left\|v_{t}\right\|^{2}\right)=\frac{\mathrm{E}\left\|w^{*}\right\|^{2}}{2\eta T}+\frac{\eta}{2}\frac{1}{T}\sum_{t=1}^{T}\mathrm{E}\left\|v_{t}\right\|^{2}$$

□

Note 16. The upper bound in (3.1) depends on the variation of v_t as

$$\mathrm{E}\left\|v_{t}\right\|^{2}=\sum_{j=1}^{d}\mathrm{Var}\left(v_{t,j}\right)+\sum_{j=1}^{d}\left(\mathrm{E}\left(v_{t,j}\right)\right)^{2} \tag{3.5}$$

where d is the dimension of $v_t=\left(v_{t,1},...,v_{t,d}\right)^{\top}$. The second term on the right hand side of (3.5) is constant as $v_{t,j}$ is the unbiased estimator of the sub-gradient by construction.

Proposition 17. *(Cont. Proposition 15) Let $f(\cdot)$ be a convex function, and let $\mathcal{H}=\{w\in\mathbb{R}:\|w\|\leq B\}$. Let $E\|v_t\|^2\leq\rho^2$. Assume we run SGD algorithm of $f(\cdot)$ with learning rate $\eta_t=\sqrt{\frac{B^2}{\rho^2T}}$ for T steps, and output $w_{\mathrm{SGD}}^{(T)}=\frac{1}{T}\sum_{t=1}^{T}w^{(t)}$. Then*

(1) *upper bound on the sub-optimality is*

$$\mathrm{E}\left(f\left(w_{\mathrm{SGD}}^{(T)}\right)\right)-f\left(w^{*}\right)\leq\frac{B\rho}{\sqrt{T}} \tag{3.6}$$

(2) *a given level of accuracy ε such that $E\left(f\left(w_{SGD}^{(T)}\right)\right)-f\left(w^{*}\right)\leq\varepsilon$ can be achieved after T iterations*

$$T\geq\frac{B^{2}\rho^{2}}{\varepsilon^{2}}.$$

Proof. It follows from Proposition 15. Condition $\mathrm{E}\left\|v_t\right\|^2 \leq \rho^2$ can be achieved, for instance by assuming Lipschitz (See Lemma 26 from "Handout 4: Gradient descent"). □

4. Stochastic gradient descent with projection

Note 18. Consider the scenario in Problem 1 where the learning problem requires to discover w^* in the restricted/bounded set $\mathcal{H}$. Assume the function to be minimized is convex in the restricted hypothesis set $\mathcal{H}$, e.g. $\mathcal{H} = \{w : \|w\| \leq B\}$, but non-convex in $\mathbb{R}^d$. Direct implementation of vanilla SGD (Algorithm 6) may produce a chain stepping out $\mathcal{H}$ and hence an output $w_{\mathrm{SGD}} \notin \mathcal{H}$. SGD can be modified to address this issue, as in Algorithm 19, by including a projection step guaranteeing $w \in \mathcal{H}$.

Algorithm 19. *Stochastic Gradient Descent with learning rate $\eta_t > 0$ and with projection in $\mathcal{H}$ for Problem 5*

For $t = 1, 2, 3, ...$ iterate:

(1) *compute*

$$w^{\left(t+\frac{1}{2}\right)} = w^{(t)} - \eta_t v_t, \tag{4.1}$$

where v_t is a random vector such that $E\left(v_t | w^{(t)}\right) \in \partial f\left(w^{(t)}\right)$

(2) *compute*

$$w^{(t+1)} = \arg\min_{w \in \mathcal{H}} \left(\left\| w - w^{\left(t+\frac{1}{2}\right)} \right\| \right) \tag{4.2}$$

(3) *terminate if a termination criterion is satisfied*

Note 20. The analysis in Section 3 holds for the SGD with projection after a slight modification in the math proofs; see Exercise 13 from the Exercise sheet.

5. Implementation of SGD in the learning Problem 1

Note 21. Proposition 22 allows a convenient implementation of SGD to the learning problem (Problem 1).

Proposition 22. *For a randomly drawn example $z \sim g(\cdot)$, the sub-gradient v of $\ell(w, z)$ at point w is an unbiased estimator of the sub-gradient of the risk $R_g(w)$ at point w.*

Proof. Let v be a sub-gradient of $\ell(w, z)$ at point w, then

$$\ell(u, z) - \ell(w, z) \geq \langle u - w, v \rangle \tag{5.1}$$

It is

$$\begin{aligned} R_g(u) - R_g(w) &= \mathrm{E}_{z \sim g}\left(\ell(u, z) - \ell(w, z) | w\right) \geq \mathrm{E}_{z \sim g}\left(\langle u - w, v \rangle | w\right) \\ &= \langle u - w, \mathrm{E}_{z \sim g}(v | w) \rangle \end{aligned}$$

Hence, by definition, v is such that $\mathrm{E}_{z \sim g}(v | w)$ is a sub-gradient of $R_g(w)$. □

Example 23. Consider that loss ℓ is differentiable wrt w. If $v = \nabla_w \ell(w, z)$, then

Note 24. Assume there is available a finite dataset $\mathcal{S}_n = \{z_i; i = 1, ..., n\}$ of size n which consists of independent realizations z_i from the data generating distribution g; $z_i \overset{\text{ind}}{\sim} g$. Batch SGD (Algorithm 25) is an implementation of the SGD (Algorithm 6) in the learning Problem 1.

Algorithm 25. *Batch Stochastic Gradient Descent with learning rate $\eta_t > 0$, and batch size m, for Problem 1.*

For $t = 1, 2, 3, ...$ iterate:

(1) *get a random sub-sample $\left\{\tilde{z}_j^{(t)}; j = 1, ..., m\right\}$ of size m with or without replacement from the complete data-set $\mathcal{S}_n$.*

(2) *compute*

$$w^{(t+1)} = w^{(t)} - \eta_t v_t, \tag{5.2}$$

where $v_t = \frac{1}{m}\sum_{j=1}^{m} \tilde{v}_{t,j}$ and $\tilde{v}_{t,j} \in \partial_w \ell\left(w^{(t)}, \tilde{z}_j^{(t)}\right)$.

(3) *terminate if a termination criterion is satisfied*

Note 26. Step 1 can be described equivalently as

(1) Randomly generate a set $\mathcal{J}^{(t)} \subseteq \{1, ..., n\}^m$ of m indices from 1 to n with or without replacement, and set a $\tilde{\mathcal{S}}_m = \left\{z_i; i \in \mathcal{J}^{(t)}\right\}$.

Hence $v_t = \frac{1}{m}\sum_{j \in \mathcal{J}^{(t)}} v_{t,j}$ where $\tilde{v}_{t,j} \in \partial_w \ell\left(w^{(t)}, z_j\right)$.

Note 27. If it is possible to sample anytime fresh examples z_i directly from the data generation model g instead of just having access to only a given finite dataset of examples $\mathcal{S}_n$, then step 1 in Algorithm 25 can become

(1) sample $\tilde{z}_j^{(t)} \sim g(\cdot)$ for $j = 1, ..., m$.

Definition 28. Online Stochastic gradient descent is the special case of Algorithm 25 using sub-samples of size one ($m = 1$), namely, only one example is randomly chosen in Step 1 of Algorithm 25.

Note 29. In theory, using larger batch size m has the benefit that reduces the variance of v_t at iteration t due to averaging effect, stabilizes the SGD algorithm, and reduces the error bound (3.1); see Remark 16.

Note 30. In practice, for a given fixed computational time, using smaller batch size m has the benefit that the algorithm iterates faster as each iteration processes less number of examples. E.g., consider the extreme cases GD vs online SGD utilized in a scenario of big-data (large training data set): if the dataset consists of several replications of the same values, GD (using all the data) has to process the same information multiple times, while the online SGD (using only one example at a time) would avoid this issue.

Note 31. In practice, for a given fixed computational time, it is possible for a batch SGD with smaller batch size m to present better generalization properties (wrt the theoretical assumptions) than those with larger m (GD is included). It is observed for the former to be often less prone to getting stuck in shallow local minima because of the additional amount of "noise" E.g., consider the extreme cases GD vs online SGD in a scenario with non-convex risk function (e.g. our theoretical assumptions as violated): if the Risk function presents local minima, considering less examples randomly chosen each time may cause fluctuations in the gradient that allow the chain to accidentally jump/escape to an area with a lower minimum.

Proposition 32. *(Implementing Proposition 17) Consider a convex-Lipschitz-bounded problem $(\mathcal{H}, \mathcal{Z}, \ell)$ with parameters ρ and B. Then for every $\epsilon > 0$, if we run SGD Algorithm 6 to minimize Problem 1 for $T \geq \frac{B^2}{\epsilon^2}\rho^2$ iterations then it produces output $w_{SGD}^{(T)}$ satisfying*

$$E\left(R_g\left(w_{SGD}^{(T)}\right)\right) \leq \min_{\forall w \in \mathcal{H}} \left(R_g\left(w\right)\right) + \epsilon$$

and hence we can achieve PAC guarantees.

Proof. It is just re-writing the formula in part 2 of Proposition 17. Notice that here, condition $\mathrm{E}\left\|v_t\right\|^2 \leq \rho^2$ is satisfied by the self-bounding property from Lipschitzness of the loss (see Lemma 26 from "Handout 4: Gradient descent"); i.e. if ℓ is ρ-Lipschitz, then $\|v_t\| \leq \rho$ where $v_t \in \partial_w \ell\left(w^{(t)}, \tilde{z}_j^{(t)}\right)$. □

Example 33. We continue Example 33 in Section 5 of Handout 4. Recall, we considered a hypothesis space $\mathcal{H}$ of linear functions $h : \mathbb{R}^2 \to \mathbb{R}$ with $h\left(w\right) = w_1 + w_2 x$, $w = \left(w_1, w_2\right)^\top$, and $\ell\left(w, z = \left(x, y\right)^\top\right) = \left(y_i - w_1 - w_2 x\right)^2$. Here we consider a big dataset $\mathcal{S}_n = \{z_1, ..., z_n\}$ with $n = 10^6$ examples.

The batch SGD algorithm (Algorithm 25) with learning rate η_t and batch size $m = 10$ is

- For $t = 1, 2, 3, ...$ iterate:
  (1) Randomly generate a set $\mathcal{J}^{(t)}$ by drawing $m = 10$ numbers from $\left\{1, ..., n = 10^6\right\}$, and set $\tilde{\mathcal{S}}_m = \left\{z_i; i \in \mathcal{J}^{(t)}\right\}$
  (2) compute
  $$w^{(t+1)} = w^{(t)} - \eta_t v_t,$$
  where
  $$v_t = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} x_j - 2\frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} y_j \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} x_j^2 - 2 \sum_{j \in \mathcal{J}^{(t)}} y_j x_j \end{pmatrix}$$
  ,
  (3) if $t \geq T = 1000$ STOP

because

$$v_t = \frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} \nabla \ell\left(w^{(t)}, \tilde{z}^{(t)}\right) = ... = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} x_j - 2\frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} y_j \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \frac{1}{m} \sum_{j \in \mathcal{J}^{(t)}} x_j^2 - 2 \sum_{j \in \mathcal{J}^{(t)}} y_j x_j \end{pmatrix}$$

In Figures A.1a & A.1d, we observe that increasing the batch size has improved the convergence however this is not a panacea. Also it had reduced the oscillations of chain $\left\{w^{(t)}\right\}$.

Example 34. Consider a (rather naive) loss function $\ell(w, z=(x,y)) = -\cos(0.5(y - w_1 - w_2 x))$, a hypothesis class $\mathcal{H} = \left\{w \in \mathbb{R}^2 : \|w\| \leq 1.5\right\}$, and assume that inputs x in dataset $\mathcal{D}$ are such that $x \in [-1, 1]$. Note that $-\cos(\cdot)$ is convex in $[-1.5, 1.5]$ and non-convex in $\mathbb{R}$. Consider learning rate $\eta_t = 50/t$ reducing to zero, and seed $w^{(0)} = (1.5, 1.5)$. An unconstrained SGD may produce a minimizer/solution outside $\mathcal{H}$ because η_t is too large at the first few iterations. We can design the online SGD (batch size $m = 1$) with projection to $\mathcal{H}$ as

- For $t = 1, 2, 3, ...$ iterate:
  (1) randomly generate a set $\mathcal{J}^{(t)} = \{j^*\}$ by drawing one number from $\left\{1, ..., n = 10^6\right\}$, and set $\tilde{\mathcal{S}}_1 = \{z_{j^*}\}$
  (2) compute

$$w^{(t+1/2)} = w^{(t)} - \frac{25}{t}\begin{pmatrix} \sin\left(0.5\left(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}\right)\right) \\ \sin\left(0.5\left(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}\right)\right) x_{j^*} \end{pmatrix}$$

$$w^{(t+1/2)} = \underset{\|w\| \leq 1.5}{\arg\min}\left(\left\|w - w^{(t+1/2)}\right\|\right)$$

  (3) if $t \geq T = 1000$ STOP

  because

$$v_t = \nabla \ell\left(w^{(t)}, z_{j^*}\right) = \begin{pmatrix} \frac{\partial}{\partial w_1^{(t)}} \ell\left(w^{(t)}, z_{j^*}\right) \\ \frac{\partial}{\partial w_2^{(t)}} \ell\left(w^{(t)}, z_{j^*}\right) \end{pmatrix} = \begin{pmatrix} 0.5 \sin\left(0.5\left(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}\right)\right) \\ 0.5 \sin\left(0.5\left(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}\right)\right) x_{j^*} \end{pmatrix}$$

  In Figures A.1b & A.1e, we observe that the SGD got trapped outside $\mathcal{H}$ due to the unreasonably large learning rate at the beginning of the iterations, while the SGD with projection step managed to stay in $\mathcal{H}$ and converge.

6. Stochastic Variance Reduced Gradient (SVRG) Ref [3]

Remark 35. Recall the upper bound of the error (3.1) in SGD depends on the variance of the stochastic gradient, as shown in (3.5) of Remark 16. Hence the algorithm may be improved by reducing the variance of each element of v_t.

Remark 36. Control variate is a general way to perform variance reduction. Let random variables $v \in \mathbb{R}$, and $y \in \mathbb{R}$. Let $z = v + c(y - \mathrm{E}(y))$ for some constant $c \in \mathbb{R}$. It is $\mathrm{E}_c(z) = \mathrm{E}(v)$ and

$$\mathrm{Var}_c(z) = \mathrm{Var}(v) + c^2 \mathrm{Var}(y) + 2c\mathrm{Cov}(x, y)$$

which is minimized for

$$c^* = -\frac{\mathrm{Cov}(v, y)}{\mathrm{Var}(y)}$$

hence

$$\mathrm{Var}_{c^*}(z) = \mathrm{Var}(v) - \frac{(\mathrm{Cov}(v, y))^2}{\mathrm{Var}(y)}$$

Note 37. For simplicity, SVRG is presented in the case where $c = 1$ and the loss function $\ell(w, z)$ is differentiable wrt w at every z hence its gradient exists. However it is applicable to the more general cases introduced.

Remark 38. Every κ iterations, SVRG keeps a snapshot $\tilde{w}$, and computes the gradient using all data i.e. $\frac{1}{n}\sum_{i=1}^{n}\ell\left(\tilde{w},z_i\right)$. At each iteration t, the update is

$$w^{(t+1)}=w^{(t)}-\eta_t\underbrace{\left[\underbrace{\nabla\ell\left(w^{(t)},\tilde{z}^{(t)}\right)}_{=v}-\underbrace{1}_{=c}\underbrace{\left(\nabla\ell\left(\tilde{w},\tilde{z}^{(t)}\right)-\frac{1}{n}\sum_{i=1}^{n}\nabla\ell\left(\tilde{w},z_i\right)\right)}_{y}\right]}_{z}$$

given that a random $\tilde{z}^{(t)}$ has been collected from the sample. The symbols below the brackets are given with reference to Remark 36.

Algorithm 39. *Stochastic Variance Reduced Gradient with learning rate $\eta_t>0$ for Problem 1.*

For $t=1,2,3,...$ iterate:

(1) *randomly get an example $\tilde{z}^{(t)}$ from S_n.*

(2) *compute*

$$w^{(t+1)}=w^{(t)}-\eta_t\left[\nabla\ell\left(w^{(t)},\tilde{z}^{(t)}\right)-\nabla\ell\left(\tilde{w},\tilde{z}^{(t)}\right)+\frac{1}{n}\sum_{i=1}^{n}\nabla\ell\left(\tilde{w},z_i\right)\right] \tag{6.1}$$

(3) *if modulo $(t,\kappa)=0$, set $\tilde{w}=w^{(t)}$*

(4) *if a termination criterion is satisfied STOP*

Remark 40. Iterations of SVRG are computationally faster than those of full GD, but SVRG can still match the theoretical convergence rate of GD.

Remark 41. How often we get snapshots, aka κ, in Algorithm 39 is specified by the researcher. The smaller the κ, the more frequent snapshots, and the more correlated the baseline y will be with the objective x and hence the bigger the performance improvement; however the iterations will be slower.

Example 42. The SVRG with learning rate $\eta_t>0$ and batch size $m=1$ is

- For $t=1,2,3,...$ iterate:
  (1) randomly generate a set $\mathcal{J}^{(t)}=\{j^*\}$ by drawing one number j^* from $\left\{1,...,n=10^6\right\}$, and set $\tilde{\mathcal{S}}_1=\{z_{j^*}\}$
  (2) compute

$$w^{(t+1)}=\begin{bmatrix}w_1^{(t)}\\w_2^{(t)}\end{bmatrix}-\eta_t\left(\begin{bmatrix}2\left(w_1^{(t)}-\tilde{w}_1^{(t)}\right)+2\left(w_2^{(t)}-\tilde{w}_2^{(t)}\right)x_{j^*}\\2\left(w_2^{(t)}-\tilde{w}_2^{(t)}\right)x_{j^*}+2\left(w_2^{(t)}-\tilde{w}_2^{(t)}\right)\left(x_{j^*}\right)^2\end{bmatrix}+\nabla\hat{R}_{\mathcal{D}}\left(\tilde{w}\right)\right) \tag{6.2}$$

  (3) if modulo $(t,\kappa)=0$,
    (a) set $\tilde{w}=w^{(t)}$

(b) compute

$$\frac{1}{n}\sum_{i=1}^{n}\ell\left(\tilde{w},z_i\right)=\begin{pmatrix}2\tilde{w}_1^{(t)}+2\tilde{w}_2^{(t)}\bar{x}-2\bar{y}\\ 2\tilde{w}_1^{(t)}\bar{x}+2\tilde{w}_2^{(t)}\overline{x^2}-2y^\top x\end{pmatrix}=\nabla\hat{R}_{\mathcal{D}}\left(\tilde{w}\right) \tag{6.3}$$

(4) if a termination criterion is satisfied STOP

Because (6.3) is actually the gradient of the Risk function at $\tilde{w}$ and

$$\nabla\ell\left(w^{(t)},z_{j^*}\right)-\nabla\ell\left(\tilde{w},z_{j^*}\right)=\begin{pmatrix}2\left(w_1^{(t)}-\tilde{w}_1^{(t)}\right)+2\left(w_2^{(t)}-\tilde{w}_2^{(t)}\right)x_{j^*}\\ 2\left(w_2^{(t)}-\tilde{w}_2^{(t)}\right)x_{j^*}+2\left(w_2^{(t)}\left(x_{j^*}\right)^2-\tilde{w}_2^{(t)}\left(x_{j^*}\right)^2\right)\end{pmatrix}$$

In Figure A.1c we observe the frequency of the snapshots has improved the convergence; however this is not a panacea as seen in Figure A.1f.

7. Preconditioned SGD; The AdaGrad algorithm

Ref [4]

Remark 43. All SGD (introduced earlier) are first order methods in the sense they consider only the gradient. Their advantage is each iteration is fast. The disadvantage is that they ignore the curvature of the space and hence can be slower to converge in cases the curvature changes eg. among dimensions of w.

Remark 44. To address this, SGD (Algorithm 6) can be modified in the update step as in Algorithm 45 by using a preconditioner P_t that accounts for the curvature (or geometry in general of f).

Algorithm 45. *Preconditioned Stochastic Gradient Descent with learning rate $\eta_t > 0$, and preconditioner P_t for the solution of the minimization problem (2.1)*

For $t=1,2,3,...$ iterate:

(1) *compute*

$$w^{(t+1)}=w^{(t)}-\eta_t P_t v_t, \tag{7.1}$$

where v_t is a random vector such that $E\left(v_t|w^{(t)}\right)\in\partial f\left(w^{(t)}\right)$, and P_t is a preconditioner

(2) *terminate if a termination criterion is satisfied, e.g.*

If $t\geq T$ then STOP

Remark 46. A natural choice of P_t can be $P_t:=\left[H_t+\epsilon I_d\right]^{-1}$, where H_t is the Hessian matrix $[H_t]_{i,j}=\frac{\partial^2}{\partial w_i\partial w_j}f\left(w\right)\Big|_{w=w^{(t)}}$ (ie. the gradient of the gradient's elements), and ϵ is a tiny $\epsilon>0$ to mitigate machine error when Hessian elements are close to zero.

Remark 47. If the preconditioner P_t is set to be the inverse of the full Hessian, it may be too expensive to perform matrix operations in (7.1) with the full Hessian, and such operations can be too unstable/inaccurate due to the random error induced by the stochasticity of the gradient.

7.1. Adaptive Stochastic Gradient Decent (AdaGrad).

Remark 48. AdaGrad aims to dynamically incorporate knowledge of the geometry of function $f(\cdot)$ (to be minimized) in earlier iterations to perform more informative gradient-based learning.

Remark 49. AdaGrad aims to perform larger updates (i.e. high learning rates) for those dimensions of w that are related to infrequent features (largest partial derivative) and smaller updates (i.e. low learning rates) for frequent ones (smaller partial derivative).

Remark 50. Hence, this strategy often improves convergence performance over standard stochastic gradient descent in settings where the data are sparse and sparse features w's are more informative.

Algorithm 51. *Adaptive Stochastic Gradient Decent (AdaGrad) can be presented in terms of preconditioned SGD (Algorithm 45) with preconditioner* $P_t = [diag(G_t) + \epsilon I_d]^{-1/2}$ *in (7.1)*

$$w^{(t+1)} = w^{(t)} - \eta_t \left[diag(G_t) + \epsilon I_d\right]^{-1/2} v_t, \tag{7.2}$$

where notation $diag(A)$ *denotes a* $d \times d$ *matrix whose diagonal is the* d *dimensional diagonal vector* $(A_{1,1}, A_{2,2}..., A_{d,d})$ *of* $d \times d$ *matrix* A *and whose off-diagonal elements are zero,* $G_t = \sum_{\tau=1}^{t} v_\tau^\top v_\tau$ *is the sum of the outer products of the gradients* $\{v_\tau; \tau \leq t\}$ *up to the state* t*, and* $\epsilon > 0$ *is a tiny value (eg,* 10^{-6}*) set for computational stability is case the gradient becomes too close to zero.*

Remark 52. AdaGrad algorithm individually adapts the learning rate of each dimension of w_t by scaling them inversely proportional to the square root of the sum of all the past squared values of the gradient $\{v_\tau; \tau \leq t\}$. This is because

$$[G_t]_{j,j} = \sum_{\tau=1}^{t} (v_{\tau,j})^2 \tag{7.3}$$

where j denotes the j-th dimension of w. Hence (7.2) and (7.2)imply that the j-th dimension of w is updated as

$$w_j^{(t+1)} = w_j^{(t)} - \eta_t \frac{1}{\sqrt{[G_t]_{j,j} + \epsilon}} v_{t,j}.$$

Remark 53. The accumulation of positive terms in (7.3) makes the sum keep growing during training and causes the learning rate to shrink and becoming infinitesimally small. This offers an automatic way to choose a decreasing learning rate simplifying setting the learning rate; however it may result in a premature and excessive decrease in the effective learning rate. This can be mitigated by still considering in (7.2) a (user specified rate) $\eta_t \geq 0$ and tuning it properly via pilot runs.

Example 54. The AdaGrad with $\eta_t = 1$, $\epsilon = 10^{-6}$, and batch size $m = 1$ is

- Set $G_0 = (0, 0)^\top$.
- For $t = 1, 2, 3, ...$ iterate:
  (1) randomly generate a set $\mathcal{J}^{(t)} = \{j^*\}$ by drawing one number from $\{1, ..., n = 10^6\}$, and set $\tilde{\mathcal{S}}_1 = \{z_{j^*}\}$

(2) compute

$$
\begin{aligned}
v_t =& \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} x_{j^*} - 2y_{j^*} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} x_{j^*}^2 - 2y_{j^*} x_{j^*} \end{pmatrix} \\
G_t =& G_{t-1} + \begin{pmatrix} v_{t,1}^2 \\ v_{t,2}^2 \end{pmatrix} \\
w^{(t+1)} =& \begin{pmatrix} w_1^{(t)} - \frac{\eta_t}{\sqrt{G_{t,1}+\epsilon}} v_{t,1} \\ w_2^{(t)} - \frac{\eta_t}{\sqrt{G_{t,2}+\epsilon}} v_{t,2} \end{pmatrix},
\end{aligned}
$$

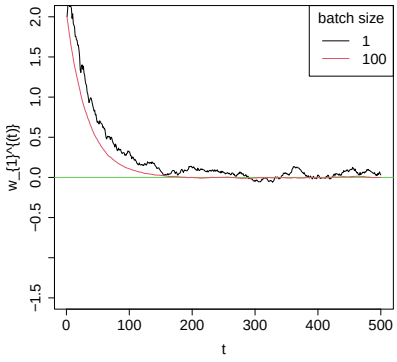
(3) if $t \geq T = 1000$ STOP

because

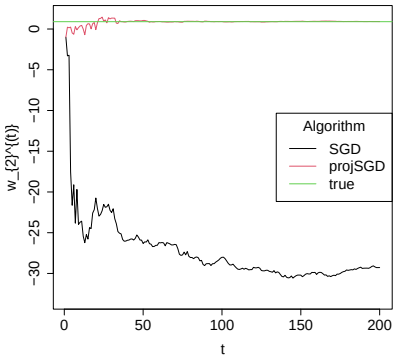
$$
v_t = \nabla \ell \left(w^{(t)}, z_{j^*} \right) = \begin{pmatrix} \frac{\partial}{\partial w_1^{(t)}} \ell \left(w^{(t)}, z_{j^*} \right) \\ \frac{\partial}{\partial w_2^{(t)}} \ell \left(w^{(t)}, z_{j^*} \right) \end{pmatrix} = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} x_{j^*} - 2y_{j^*} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} x_{j^*}^2 - 2y_{j^*} x_{j^*} \end{pmatrix}
$$

In Figures A.1g & A.1h, we see that AdaGrad with $\eta = 1$ works (I did not try to tune it), however to make vanilla SGD to work I have to tune $\eta = 0.03$ otherwise for $\eta = 1.0$ it did not work.

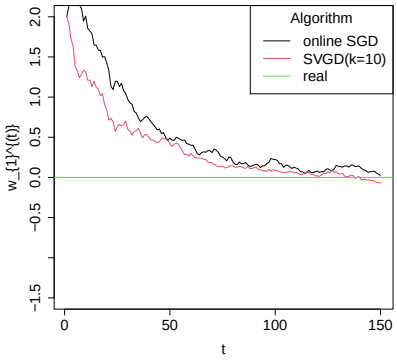
Appendix A. Plots



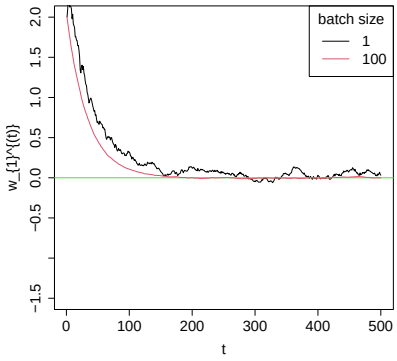
(A) batch SGD Example 33 w_1



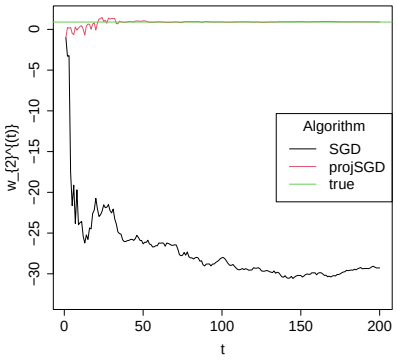
(B) online SGD with projection Example 34w_1



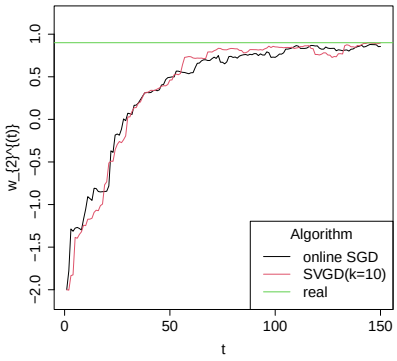
(C) SVRG Example 42 w_1



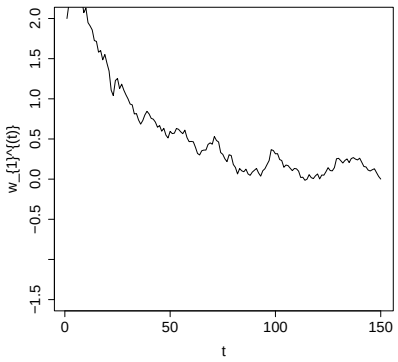
(D) batch SGD Example 33 w_2



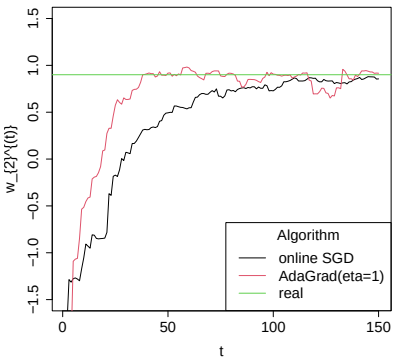
(E) online SGD with projection Example 34 w_2



(F) SVRG Example 42 w_2



(G) online AdaGrad Example 54w_1



(H) online AdaGrad Example 54w_2

FIGURE A.1. Simulations of the Examples

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Handout 6: Bayesian Learning via Stochastic gradient and Stochastic gradient Langevin dynamics

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Aim. To introduce the Bayesian Learning, and Stochastic gradient Langevin dynamics (description, heuristics, and implementation). Stochastic gradient descent will be implemented in the Bayesian learning too.

Reading list & references:

(1) Welling, M., & Teh, Y. W. (2011). Bayesian learning via stochastic gradient Langevin dynamics. In Proceedings of the 28th international conference on machine learning (ICML-11) (pp. 681-688).
(2) Bottou, L. (2012). Stochastic gradient descent tricks. In Neural networks: Tricks of the trade (pp. 421-436). Springer, Berlin, Heidelberg.
(3) Sato, I., & Nakagawa, H. (2014). Approximation analysis of stochastic gradient Langevin dynamics by using Fokker-Planck equation and Ito process. In International Conference on Machine Learning (pp. 982-990). PMLR.
(4) Teh, Y. W., Thiery, A. H., & Vollmer, S. J. (2016). Consistency and fluctuations for stochastic gradient Langevin dynamics. Journal of Machine Learning Research, 17.
(5) Vollmer, S. J., Zygalakis, K. C., & Teh, Y. W. (2016). Exploration of the (non-) asymptotic bias and variance of stochastic gradient Langevin dynamics. The Journal of Machine Learning Research, 17(1), 5504-5548. –>further reading for theory
(6) Nemeth, C., & Fearnhead, P. (2021). Stochastic gradient Markov chain Monte Carlo. Journal of the American Statistical Association, 116(533), 433-450.

1. Bayesian learning and motivations

Note 1. Bayesian methods are appealing in their ability to capture uncertainty in learned parameters and avoid overfitting. Arguably with large datasets there will be little overfitting. Alternatively, as we have access to larger datasets and more computational resources, we become interested in building more complex models (eg from a logistic regression to a deep neural network), so that there will always be a need to quantify the amount of parameter uncertainty.

Note 2. Consider a Bayesian statistical model with sampling distribution (statistical model) $f(z|w)$ labeled by an unknown parameter $w \in \Theta \subseteq \mathbb{R}^d$ that follows a prior distribution $f(w)$. Assume a dataset $\mathcal{S}_n = \{z_i; i = 1, ..., n\}$ of size n containing independently drawn examples. Let $L_n(w) := f(z_{1:n}|w)$ denote the likelihood of the observables $\{z_i \in \mathcal{Z}\}_{i=1}^n$ give parameter w. The Bayesian

model is denoted as

$$\begin{cases} z_i|w & \overset{\text{ind}}{\sim} f\left(z_{1:n}|w\right), \ i=1,...,n \\ w & \sim f\left(w\right) \end{cases} \tag{1.1}$$

Note 3. With regards to the Bayesian model in Note 2, we denote the likelihood of the observables $\{z_i \in \mathcal{Z}\}_{i=1}^n$ given the parameter w as

$$L_n\left(w\right) := f\left(z_{1:n}|w\right) = \prod_{i=1}^{n} f\left(z_i|w\right)$$

Note 4. Bayesian learning (inference) relies on the posterior distribution density

$$f\left(w|z_{1:n}\right) = \frac{L_n\left(w\right) f\left(w\right)}{\int L_n\left(w\right) f\left(w\right) \mathrm{d}w} \tag{1.2}$$

which quantifies the researcher's belief (or uncertainty) about the unknown parameter w learned given examples $\{z_i \in \mathcal{Z}\}_{i=1}^n$. It is often intractable; hence there is often a need to numerically compute it. (Section 3)

Note 5. Point estimation of a function h of w is often performed via computation of the posterior expectation w given the examples in $\mathcal{S}_n$

$$\mathrm{E}_f\left(h\left(w\right)|z_{1:n}\right) = \int h\left(w\right) f\left(w|z_{1:n}\right) \mathrm{d}w \tag{1.3}$$

It is often intractable; hence there is often a need to numerically compute it. (Section 3)

Note 6. Point estimation of w can also be performed via maximum a-posteriori (MAP) estimator w^* of w that is the maximizer w^* of (1.2) i.e.

$$w^* = \arg\max_{w\in\Theta} \left(f\left(w|z_{1:n}\right)\right) \tag{1.4}$$

$$= \arg\max_{w\in\Theta} \left(\underbrace{\log\left(L_n\left(w\right)\right)}_{\text{(I)}} + \underbrace{\log\left(f\left(w\right)\right)}_{\text{(II)}} \right) \tag{1.5}$$

Note that (I) may be interpreted as an empirical risk function, and (II) can be interpreted as a shrinkage term in terms of shrinkage methods (like LASSO, Ridge). It is often intractable; hence there is often a need to numerically compute it. (Section 2)

Note 7. To describe the learning algorithms Gradient Descent (GD), Stochastic Gradient Descent (SGD), and Stochastic Gradient Langevin Dynamics (SGLD), we consider that the examples (data) in (1.1) are independent realizations from the sampling distribution i.e. $z_i|w \sim f\left(\cdot|w\right)$ for $i=1,...,n$ and that w is continuous (not discrete).

Note 8. In what follows, we first present the implementation of GD and SGD addressing MAP learning, and then we introduce the implementation of SGLD addressing posterior density and expectation learning.

2. Maximum A Posteriori (MAP) learning via GD and SGD

Problem 9. Given the Bayesian model (1.1), and rearranging (1.4), MAP estimate w^* of w can be computed as

$$w^* = \arg\max_{w\in\Theta} \left(\log\left(L_n\left(w\right)\right) + f\left(w\right)\right) = \arg\max_{w\in\Theta} \left(\sum_{i=1}^{n} \log\left(f\left(w|z_i\right)\right) + \log\left(f\left(w\right)\right)\right) \tag{2.1}$$

Note 10. GD is particularly suitable to solve (2.1) when w has high dimensionality.

Algorithm 11. *Gradient descent (Algorithm 4 "Handout 4: Gradient descent ") with learning rate $\eta_t \geq 0$ can be used to address Problem 9 by using the update rule as*

For $t = 1, 2, 3, ...$ iterate:

(1) *Compute*

$$w^{(t+1)} = w^{(t)} + \eta_t \left(\sum_{i=1}^{n} \nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right) + \nabla_w \log\left(f\left(w^{(t)}\right)\right)\right) \tag{2.2}$$

Note 12. The implementation of other GD variants (eg (3.2) in Handout 2) is straightforward, based on Algorithm 11.

Note 13. SGD is particularly suitable to solve (2.1) when w has high dimensionality, and in big-data problems since the repetitive computation of the sum in (2.2) is prohibitively expensive. Yet consider the benefits of SGD against GD as discussed in (Remarks 27 and 28 of Handout 3).

Algorithm 14. *Batch Stochastic Gradient Descent (Algorithm 22 in "Handout 5: Stochastic gradient descent") with learning rate $\eta_t \geq 0$ and batch size m can be used to address Problem 9 by using the update rule as*

For $t = 1, 2, 3, ...$ iterate:

(1) *generate a random set $\mathcal{J}^{(t)} \subseteq \{1, ..., n\}^m$ of m indices from 1 to n with or without replacement, and set a $\tilde{\mathcal{S}}_m = \left\{z_i; i \in \mathcal{J}^{(t)}\right\}$.*

(2) *compute*

$$w^{(t+1)} = w^{(t)} + \eta_t \left(\frac{n}{m} \sum_{j\in\mathcal{J}^{(t)}} \nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right) + \nabla_w \log\left(f\left(w^{(t)}\right)\right)\right) \tag{2.3}$$

Note 15. Recursion (2.3) is justified in terms of SGD theory as

$$\mathrm{E}_{\mathcal{J}^{(t)}\sim\text{simple-random-sampling}} \left(\frac{n}{m} \sum_{j\in\mathcal{J}^{(t)}} \nabla_w \log\left(f\left(z_j|w^{(t)}\right)\right)\right) = \sum_{i=1}^{n} \nabla_w \log\left(f\left(z_i|w^{(t)}\right)\right) \tag{2.4}$$

see Exercise 11 from the Exercise sheet.

Note 16. The implementation of the SGD variants (Algorithms 22, 39, 45, 51 in Handout 3)) is straightforward based on Algorithm 14 and (2.4).

3. Fully Bayesian learning via SGLD

Problem 17. Fully Bayesian learning, computationally, is the problem of recovering the posterior distribution $f(w|z_{1:n})$ of w given $z_{1:n}$ that admits density (1.2). For a given Bayesian model (1.1), the Bayesian estimator of $h := h(w)$ can be computed as the posterior expectation of w given the data $\mathcal{S}_n$

$$\mathrm{E}_f(h(w)|z_{1:n}) = \int h(w) f(w|z_{1:n}) \,\mathrm{d}w \tag{1.3}$$

Note 18. Monte Carlo integration aims at approximating (1.3), by using Central Limit Theorem or Law of Large Numbers arguments as $\hat{h} \approx \mathrm{E}_f(h(w)|z_{1:n})$ where

$$\hat{h} = \frac{1}{T}\sum_{t=1}^{T} h\left(w^{(t)}\right) \tag{3.1}$$

where $\left\{w^{(t)}\right\}$ are T simulations drawn (approximately) from the posterior distribution 1.2. This theory is subject to conditions we skip.

Note 19. Stochastic gradient Langevin dynamics (SGLD) algorithm is able to approximately produce samples from the posterior distribution (1.2) of parameters w given the available data $z_{1:n}$. That allows to recover the whole posterior distribution (1.2) (hence account for the uncertainty in parameters) and approximate posterior expectations (1.3) by averaging out (3.1) according to the Monte Carlo integration (Remark 18).

Note 20. Stochastic gradient Langevin dynamics (SGLD) algorithm is able to generate a sample approximately distributed according to the posterior distribution (1.2). That allows to recover the whole posterior distribution (hence account for uncertainty in parameters) and approximate posterior expectations based on the Monte Carlo integration (Remark 18).

Note 21. SGLD relies on injecting the 'right' amount of noise to a standard stochastic gradient optimization recursion (2.2), such that, as the stepsize η_t properly reduces, the produced chain $\left\{w^{(t+1)}\right\}$ converges to samples that could have been drawn from the true posterior distribution.

Algorithm 22. *Stochastic Gradient Langevin Dynamics (SGLD) with learning rate $\eta_t > 0$, batch size m, and temperature $\tau > 0$ is*

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(1) *Generate a random set $\mathcal{J}^{(t)} \subseteq \{1, ..., n\}^m$ of m indices from 1 to n with or without replacement, and set a $\tilde{\mathcal{S}}_m = \left\{z_i; i \in \mathcal{J}^{(t)}\right\}$.*

(2) *Compute*

$$w^{(t+1)} = w^{(t)} + \eta_t \left(\frac{n}{m} \sum_{i \in J^{(t)}} \nabla \log f\left(z_i | w^{(t)}\right) + \nabla \log f\left(w^{(t)}\right) \right) + \sqrt{\eta_t}\sqrt{\tau}\epsilon_t \tag{3.2}$$

where $\epsilon_t \overset{\text{iid}}{\sim} \mathrm{N}(0, I)$.

(3) *Terminate if a termination criterion is satisfied; E.g., $t \leq T_{max}$ for a prespecified $T_{max} > 0$.*

Note 23. The first few iterations from Algorithm 22 involve values generated at the beginning of the running algorithm while the chain have not yet converged to (or reached) an area of substantial posterior mass. Hence they are discarded from the output of the SGLD. These values are called burn-in.

Note 24. The output of SGLD (Algorithm 22) $\left\{w^{(t)}\right\}$ includes the generated values of w produced during the last few iterations of the running algorithm (aka the end tail of the generated chain).

Note 25. SGLD (Algorithm 22) generates as output a random chain $\left\{w^{(t)}\right\}$ that is approximately distributed according to a distribution with density such as

$$f_\tau(w|z_{1:n}) \propto \exp\left(\frac{1}{\tau} \prod_{i=1}^{n} f(z_i|w) f(w) \right) \tag{3.3}$$

$$\propto \exp\left(\frac{1}{\tau} L_n(w) f(w) \right) \tag{3.4}$$

under regularity conditions. Conditions 26 on the learning rate are rather inevitable and should be satisfied.

Condition 26. Regarding the learning rate (or gain) $\{\eta_t\}$ should satisfy conditions

(1) $\eta_t \geq 0$,
(2) $\sum_{t=1}^{\infty} \eta_t = \infty$
(3) $\sum_{t=1}^{\infty} \eta_t^2 < \infty$

Note 27. The temperature parameter $\tau > 0$ is user specified and aims at controlling (eg; inflating) the variance of the produced chain for instance with practical purpose to escape from local modes (otherwise energy barriers) in non-convex problems.

Note 28. SGLD for $\tau = 1$ approximately simulates from the posterior (1.2).

Note 29. The popular learning rates $\{\eta_t\}$ in Note 10 in "Handout 4: Gradient descent " satisfy Condition 26 and hence can be used in SGD too. Once parametrized, η_t can be tuned based on pilot runs using a reasonably small number of data.

Note 30. (Mathematically speaking) The stochastic chain in (3.2) can be viewed as a discretization of the continuous-time Langevin diffusion described by the stochastic differential equation

$$\mathrm{d}W(t) = -\nabla_w \left[-\log f\left(W(t)\,|z_{1:n}\right)\right]\mathrm{d}t + \sqrt{2\tau}\mathrm{d}B(t)\,,\ t \geq 0 \tag{3.5}$$

where $\{B(t)\}$ is a standard Brownian motion[1] in $\mathbb{R}^d$ (i.e.). Under suitable assumptions on f, it can be shown that a Gibbs distribution with PDF such as

$$f^*\left(w|z_{1;n}\right) \propto \exp\left(-\frac{1}{\tau}\left[-\log f\left(W(t)\,|z_{1:n}\right)\right]\right) \tag{3.6}$$

is the unique invariant distribution of (3.5), and that the distributions of $W(t)$ converge rapidly to f^* as $t \to \infty$.

Note 31. (Heuristically speaking) In the initial phase of running, the stochastic gradient noise will dominate the injected noise ϵ_t and the algorithm will imitate an efficient SGD Algorithm 11 -but this is until η_t or $\nabla \log\left(L_n(w)\right)$ become small enough. In the later phase of running, the injected noise ϵ_t will dominate the stochastic gradient noise, so the SGLD will imitate a Langevin dynamics for the target distribution (1.2). The aim is for to the algorithm to transition smoothly between the two phases. Whether the algorithm is in the stochastic optimization phase or Langevin dynamics phase depends on the variance of the injected noise versus that of the stochastic gradient.

Note 32. One can argue that, the output of SGLD is also an "almost" minimizer of the empirical risk for large enough t. A draw from the Gibbs distribution (3.6) is approximately a minimizer of (2.1). Also one can show that the SGLD recursion tracks the Langevin diffusion (3.5) in a suitable sense. Hence, both imply that the distributions of $W(t)$ will be close to the Gibbs distribution (3.6) for all sufficiently large t.

Note 33. To guarantee the algorithm to work it is important for the step sizes η_t to decrease to zero, so that the mixing rate of the algorithm will slow down with increasing number of iterations t. Then, we can keep the step size η_t constant once it has decreased below a critical level.

Note 34. Expectation (1.3), can be estimated as an arithmetic average

$$\widehat{h_T(w)} = \frac{1}{T}\sum_{t=1}^{T} h\left(w^{(t)}\right) \tag{3.7}$$

as $\widehat{h_T(w)} \to \mathrm{E}_f\left(h(w)\,|z_{1:n}\right)$ based on LLN arguments.

Note 35. Another more efficient estimator for the expectation (1.3) is the weighted arithmetic average

$$\widehat{h(w)} = \sum_{t=T_0+1}^{T} \frac{\eta_t}{\sum_{t=T_0+1}^{T}\eta_{t'}} h\left(w^{(t)}\right) \tag{3.8}$$

[1] A a continuous-time stochastic process: (1) $B(0) = 0$; (2) $B(t)$ is almost surely continuous ; (3) $B(t)$ has independent increaments ; (4) $B(t) - B(s) \sim \mathrm{N}(0, t-s)$ for $0 \leq s \leq t$.

Because the step size η_t decreases, the mixing rate of the chain $\left\{w^{(t)}\right\}$ decreases as well and the simple sample average (3.7) will overemphasize the tail end of the sequence where there is higher correlation among the samples resulting in higher variance in the estimator.

Note 36. Certain dimensions may have a vastly larger curvature leading to much bigger gradients. In this case a symmetric preconditioning matrix $P_t > 0$ can transform all dimensions to the same scale; this is similar to the SGD case in "Handout 5: Stochastic gradient descent". Hence the update (3.2) becomes

$$w^{(t+1)} = w^{(t)} + \eta_t P_t \left(\frac{n}{m} \sum_{i \in J^{(t)}} \nabla \log f\left(z_i | w\right) + \nabla \log f\left(w\right) \right) + \sqrt{\eta_t} \sqrt{\tau} P_t^{\frac{1}{2}} \epsilon_t \tag{3.9}$$

where $P_t^{\frac{1}{2}}$ is such that $P_t^{\frac{1}{2}} \left(P_t^{\frac{1}{2}} \right)^{\top} = P_t$.

Note 37. 'Exploding gradients' is the practical phenomenon in which large updates to weights during training can cause a numerical overflow or underflow due to the machine error of the computer. Practical solutions involve, at each iteration t, checking the magnitude of the gradient v_t, (e.g., Euclidean norm $\|v_t\|$), and instantly changing it (e.g., truncating it) if it is gonna result an overflow.

Gradient scaling: involves normalizing the gradient vector such that vector norm (magnitude) equals a defined value. More formally, given any gradient v on an example, gradient clipping can be used in a standard recursion

$$w^{(t+1)} = w^{(t)} + \eta_t v_t$$

as

$$w^{(t+1)} = w^{(t)} + \eta_t \text{clip}\left(v_t, c\right)$$

where

$$\text{clip}\left(v, c\right) = v \min\left(1, \frac{c}{\|v\|}\right)$$

and c is a clipping threshold impaling that clipping will take place at iteration t if $\|v_t\| > c$.

Gradient clipping: involves forcing the gradient values (element-wise) to a specific minimum or maximum value if the gradient exceeded an expected range.

Beware that unreasonable clipping may introduce significant bias and hence it should not be applied unnecessarily.

4. Examples [2]

We continue the Example 33 in Handout 1, and Example **??** in Handout 2. Consider the Bayesian Normal linear regression model

$$\begin{cases} y_i|\beta,\sigma^2 \sim \mathrm{N}\left(x_i^\top \beta, \sigma^2\right) & \text{sampling distribution } f\left(y_i|\beta,\sigma^2\right) \\ \beta|\sigma^2 \sim \mathrm{N}\left(\mu, \sigma^2 V\right) & \text{prior } f\left(\beta|\sigma^2\right) \\ \sigma^2 \sim \mathrm{IG}\left(\phi,\psi\right) & \text{prior } f\left(\sigma^2\right) \end{cases}$$

and $f\left(\beta,\sigma^2\right) = f\left(\beta|\sigma^2\right) f\left(\sigma^2\right)$, $\beta \in \mathbb{R}^d$, and $\sigma^2 \in \mathbb{R}_+$. Note given densities

$$\begin{aligned} \mathrm{N}\left(x|\mu,\Sigma\right) &= \left(\frac{1}{2\pi}\right)^d \frac{1}{|\Sigma|} \exp\left(-\frac{1}{2}\left(x-\mu\right)^\top \Sigma^{-1}\left(x-\mu\right)\right) \\ \mathrm{IG}\left(x|a,b\right) &= \frac{b^a}{\Gamma\left(a\right)} x^{-a-1} \exp\left(-\frac{b}{x}\right) 1\left(x \geq 0\right) \end{aligned}$$

Because SGD (Algorithm 14) and SGLD (Algorithm 22) can handle cases where $w \in \mathbb{R}^d$ in a straightforward manner than what they do when $w = \left(\beta,\sigma^2\right) \in \mathbb{R}^d \times \mathbb{R}_+$ which requires an additional projection step; we consider a transformation $w = (\beta,\gamma) \in \mathbb{R}^d \times \mathbb{R}$ with $\gamma = \log\left(\sigma^2\right)$. Hence, the Bayesian model becomes

$$\begin{cases} y_i|\beta,\sigma^2 \sim \mathrm{N}\left(x_i^\top \beta, \exp\left(\gamma\right)\right) & \text{sampling distribution } f\left(y_i|\beta,\gamma\right) \\ \beta|\sigma^2 \sim \mathrm{N}\left(\mu = 0, \exp\left(\gamma\right) V\right) & \text{prior } f\left(\beta|\gamma\right) \\ \gamma \sim f_\gamma\left(\gamma\right) & \text{prior } f\left(\gamma\right) \end{cases}$$

where $f_\gamma\left(\gamma\right)$ is computed according to the method of bijective transformation of random variables; i.e.

$$f_\gamma\left(\gamma\right) = \mathrm{IG}\left(\exp\left(\gamma\right)|\phi,\psi\right)\left|\frac{\mathrm{d}}{\mathrm{d}\gamma}\exp\left(\gamma\right)\right| = \mathrm{IG}\left(\exp\left(\gamma\right)|\phi,\psi\right)\exp\left(\gamma\right)$$

Then we can compute the required gradients in order to run the SGD, and SGLD with respect to $w = (\beta,\gamma)$ with $\gamma = \log\left(\sigma^2\right)$.

$$\begin{aligned} \log\left(f\left(z_i = (x_i,y_i)|w\right)\right) =& -\frac{1}{2}\log\left(2\pi\right) - \frac{1}{2}\gamma - \frac{1}{2}\left(y_j - x_i^\top\beta\right)^2 \exp\left(-\gamma\right) \\ \log\left(f\left(w = (\beta,\gamma)\right)\right) =& \log\left(f\left(\beta|\gamma\right)\right) + \log\left(f\left(\gamma\right)\right) \\ \log\left(f\left(\beta|\gamma\right)\right) =& -\frac{d}{2}\log\left(2\pi\right) - \frac{d}{2}\gamma - \frac{1}{2}\left|V\right| - \frac{1}{2}\exp\left(-\gamma\right)\left(\beta-\mu\right)^\top V^{-1}\left(\beta-\mu\right) \\ \log\left(f\left(\gamma\right)\right) =& \psi\log\left(\phi\right) - \log\left(\Gamma\left(\phi\right)\right) - \left(\phi+1\right)\gamma - \psi\exp\left(-\gamma\right) + \gamma \end{aligned}$$

[2] Code is available from `https://github.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2023/tree/main/Lecture_handouts/code/04.Stochastic_gradient_Langevine_dynamics`

Hence for the log sampling PDF we have

$$\nabla_w \log\left(f\left(z_i|w\right)\right) = \left(\frac{\mathrm{d}}{\mathrm{d}\beta}\log\left(f\left(z_i|w\right)\right) \; ; \; \frac{\mathrm{d}}{\mathrm{d}\gamma}\log\left(f\left(z_i|w\right)\right)\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\log\left(f\left(z_i|w\right)\right) = \left(y_i - x_i^\top \beta\right) x_i \exp\left(-\gamma\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}\gamma}\log\left(f\left(z_i|w\right)\right) = -\frac{1}{2} + \frac{1}{2}\left(y_j - x_i^\top \beta\right)^2 \exp\left(-\gamma\right)$$

...so

$$\nabla_w \log\left(f\left(z_i|w\right)\right) = \begin{pmatrix} \left(y_i - x_i^\top \beta\right) x_i \exp\left(-\gamma\right) \\ -\frac{1}{2} + \frac{1}{2}\left(y_j - x_i^\top \beta\right)^2 \exp\left(-\gamma\right) \end{pmatrix} \tag{4.1}$$

Hence for the log a priori PDF we have

$$\nabla_w \log\left(f\left(w\right)\right) = \left(\frac{\mathrm{d}}{\mathrm{d}\beta}\log\left(f\left(w\right)\right) \; ; \; \frac{\mathrm{d}}{\mathrm{d}\gamma}\log\left(f\left(w\right)\right)\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\log\left(f\left(w\right)\right) = -\exp\left(-\gamma\right) V^{-1}\left(\beta - \mu\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}\gamma}\log\left(f\left(w\right)\right) = -\frac{d}{2} + \frac{1}{2}\exp\left(-\gamma\right)\left(\beta - \mu\right)^\top V^{-1}\left(\beta - \mu\right) - \left(\phi + 1\right) + \psi\exp\left(-\gamma\right) + 1$$

...so

$$\nabla_w \log\left(f\left(w\right)\right) = \begin{pmatrix} -\exp\left(-\gamma\right) V^{-1}\left(\beta - \mu\right) \\ \frac{d}{2} + \frac{1}{2}\exp\left(-\gamma\right)\left(\beta - \mu\right)^\top V^{-1}\left(\beta - \mu\right) - \left(\phi + 1\right) + \psi\exp\left(-\gamma\right) + 1 \end{pmatrix} \tag{4.2}$$

To implement SGD (Algorithm 14) and SGLD (Algorithm 22) , we just need to plug in the computed gradients (4.1) and (4.2) for $w = (\beta, \gamma) \in \mathbb{R}^d \times \mathbb{R}$ with $\gamma = \log\left(\sigma^2\right)$. After running SGD and SGLD with the computed gradients with respect to $w = (\beta, \gamma) \in \mathbb{R}^d \times \mathbb{R}$ with $\gamma = \log\left(\sigma^2\right)$, and obtaining chains $\left\{w^{(t)} = \left(\beta^{(t)}, \gamma^{(t)}\right)\right\}_{t=1}^T$, we can just perform transformation $\left\{\left(\sigma^{(t)}\right)^2 = \exp\left(\gamma^{(t)}\right)\right\}_{t=1}^T$ if we are interested in learning $\left(\beta, \sigma^2\right)$.

We consider $\mu = 0$, $\phi = 1$, $\psi = 1$, and $V = 100 I_d$, for our simulations below.

- In Figures 4.1, we ran the SGD for different batch sizes m and compared it against the exact MLE. We observe that SGD trace converges to the exact MLE. The oscillations are due to the stochastic gradient (ie, noise in the gradient).
- In Figures 4.2, we ran the SGLD for different batch sizes m but the same temperature $\tau = 1$ and compared it against the exact posterior densities. We observe that the histograms of $\left\{w^{(t)}\right\}$ produced from SGLD are closer to the curves representing the exact posteriors when the batch size m is bigger. As we said this is not a panacea; if the landscape of the exact psterior density was multimodal (aka not convex but with had several maxima), then the SGLD using smaller batch sizes could have performed better, in the sense that the inflated noise from the stochastic gradient could accidentally make the generated chain to pass the low mass barrier and visit a different mode, unlike the one with larger batch-size and hence smaller variation.

- In Figures 4.3, we ran the SGLD for different temperatures τ but the same batch sizes $m = 100$ and compared it against the exact posterior densities. We observe that increasing the temperature τ may increase the variation of the produced chain. We can use a large τ at the beginning of the run of the algorithm to perform an exploration of the space (this is particularly useful for non-convex/multimodal densities as it allows visiting different modes), and later on we can use a smaller temperature such as $\tau = 1$.

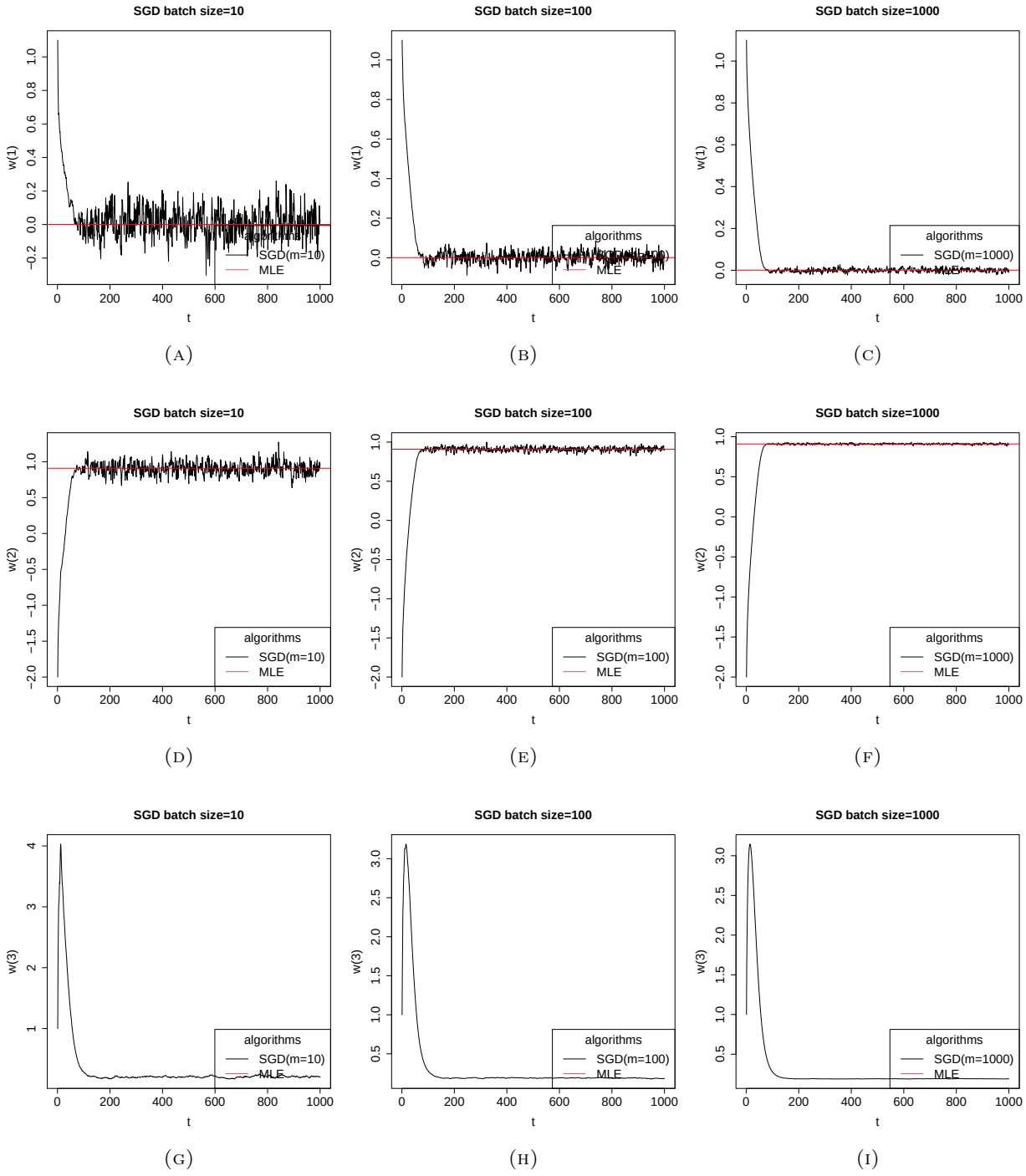

FIGURE 4.1. Bayesian learning via SGD (SGD vs (exact)MLE) Study on batch size m.

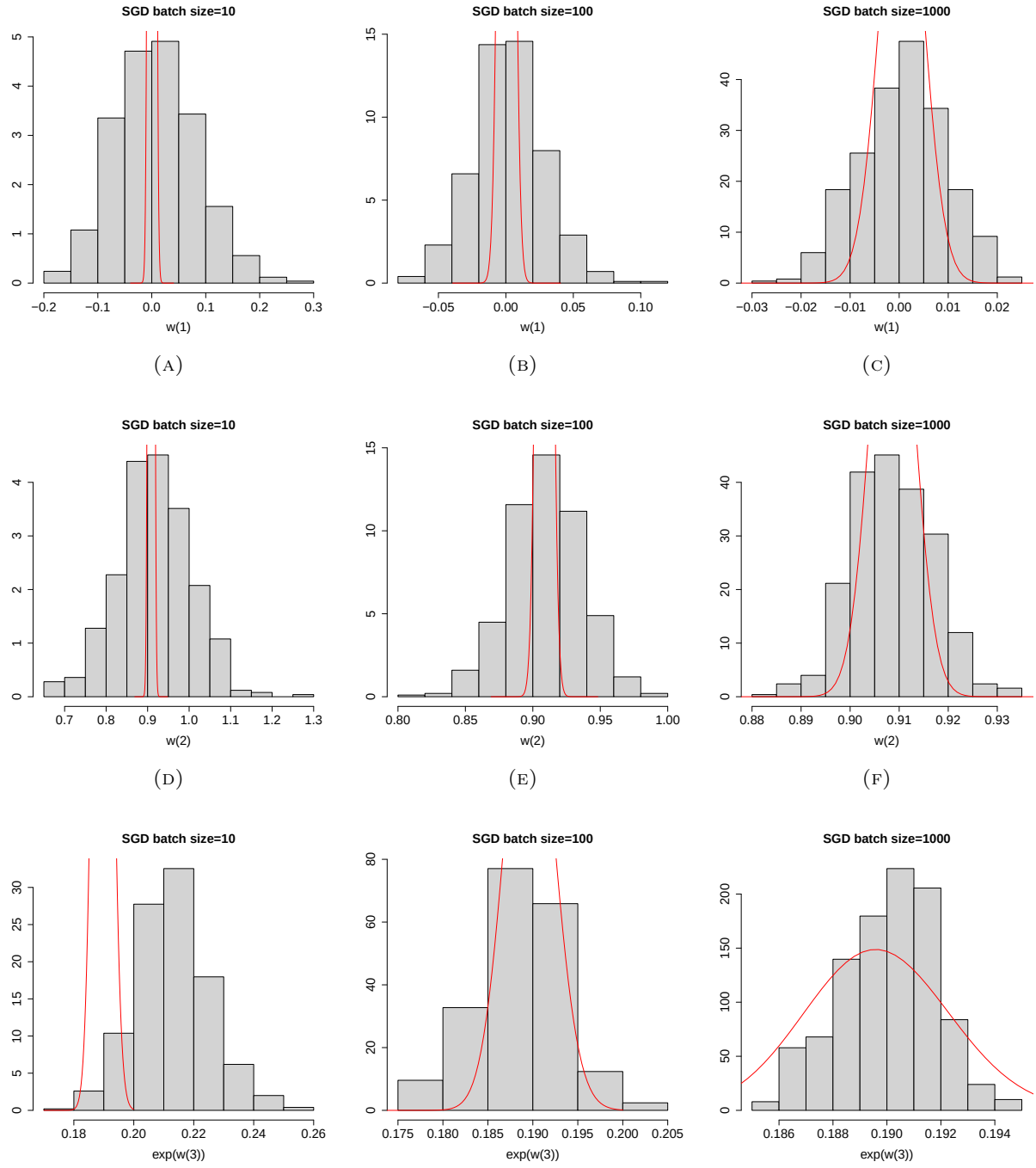

FIGURE 4.2. Bayesian learning: SGLD vs exact posterior (in red). Temperature $\tau = 1$. Study on batch size m

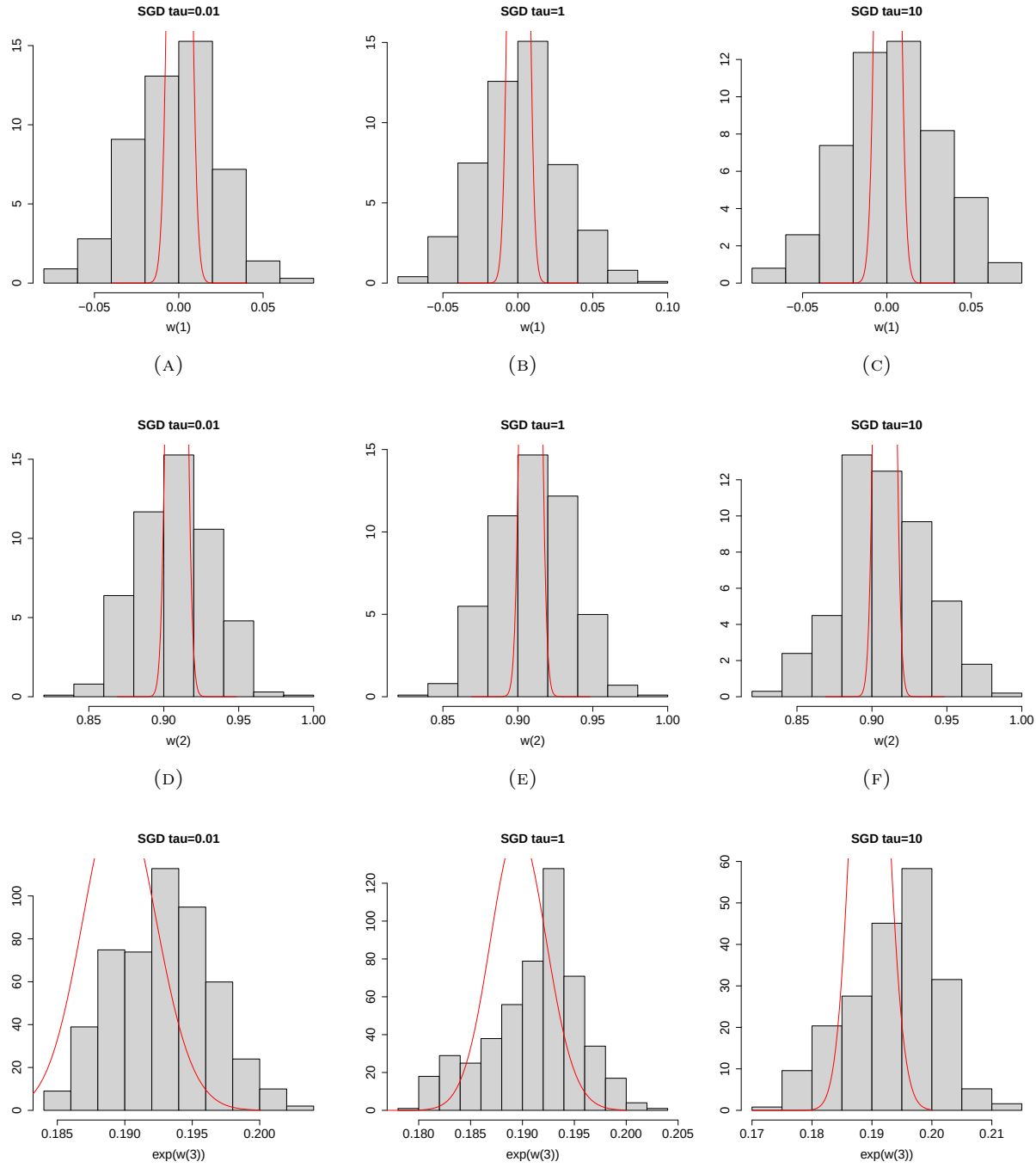

FIGURE 4.3. Bayesian learning: SGLD vs exact posterior (in red). Batch size = 100. Study on τ