

Machine Learning and Neural Networks III (MATH3431)

Epiphany term

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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-recognition>
- 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 It is very comprehensive (compared to others) and it goes deep enough for the module although it may be a bit outdated.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.
- 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.

Handout 0: Learning problem: Definitions, notation, and formulation –A recap

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

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) 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 focus here) and the unsupervised learning.

Supervised learning problems involve applications where the training data $z \in \mathcal{Z}$ comprises 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 recover 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. $x \mapsto y$. 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 $y \in \mathcal{Y}$ 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, $h : \mathcal{X} \rightarrow \mathcal{Y}$ 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 $x \rightarrow y$ where $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and $y \in \mathcal{Y} \subseteq \mathbb{R}$. Hypothesis is a linear function $h : \mathcal{X} \rightarrow \mathcal{Y}$ (that learner wishes to learn) to approximate mapping $x \rightarrow y$. The hypothesis set $\mathcal{H} = \{x \rightarrow \langle w, x \rangle : w \in \mathbb{R}^d\}$. We can use the loss $\ell(h, (x, y)) = (h(x) - y)^2$.

Definition 4. Training data set \mathcal{S} of size m is any finite sequence of pairs $((x_i, y_i) ; i = 1, \dots, m)$ in $\mathcal{X} \times \mathcal{Y}$. This is the information that the learner has assess.

Definition 5. 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.

Definition 6. We denote as $\mathfrak{A}(\mathcal{S})$ the hypothesis (outcome) that a learning algorithm \mathfrak{A} returns given training sample \mathcal{S} .

Definition 7. (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 $\ell : \mathcal{H} \times \mathcal{Z} \rightarrow \mathbb{R}_+$. The purpose of loss function $\ell(h, z)$ is to quantify the "error" for a given hypothesis h and example z –the greater the error the greater its value of the loss.

Example 8. (Cont. Example 3) In regression problems $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ and $\mathcal{Y} \subset \mathbb{R}$ is uncountable, a loss function can be

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

Example 9. In binary classification problems with $h : \mathcal{X} \rightarrow \mathcal{Y}$ a learner where $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ and $\mathcal{Y} = \{0, 1\}$ is discrete, a loss function can be

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

Definition 10. (Risk function) The risk function $R_g(h)$ of h is the expected loss of the hypothesis $h \in \mathcal{H}$, w.r.t. probability distribution g over domain \mathcal{Z} ; i.e.

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

Remark 11. In learning, an ideal way to obtain an optimal predictor h^* is to compute the risk minimizer

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

¹ $\langle w, x \rangle = w^\top x$

Example 12. (Cont. Ex. 8) The risk function is $R_g(h) = \mathbb{E}_{z \sim g} (h(x) - y)^2$, and it measures the quality of the hypothesis function $h : \mathcal{X} \rightarrow \mathcal{Y}$, (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 from h and the true target values y at every x .

Note 13. 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 resort to the Empirical risk function.

Definition 14. (Empirical risk function) The empirical risk function $\hat{R}_S(h)$ of h is the expectation of loss of h over a given sample $S = (z_1, \dots, z_m) \in \mathcal{Z}^m$; i.e.

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

Example 15. (Cont. Example 12) Given given sample $S = \{(x_i, y_i); i = 1, \dots, m\}$ the empirical risk function is $\hat{R}_S(h) = \frac{1}{m} \sum_{i=1}^m (h(x_i) - y_i)^2$.

Example 16. 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

$$(2.2) \quad R_g(\theta) = \mathbb{E}_{z \sim g} \left(\log \left(\frac{g(z)}{f_\theta(z)} \right) \right) = \mathbb{E}_{z \sim g} (\log(g(z))) - \mathbb{E}_{z \sim g} (\log(f_\theta(z)))$$

whose minimizer is

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

as the first term in (2.2) is constant. Note that in the Maximum Likelihood Estimation technique the MLE θ_{MLE} is the minimizer of

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

where $S = \{z_1, \dots, z_m\}$ 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 17. 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 18. Consider the multiple linear regression problem $x \mapsto y$ where $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and $y \in \mathcal{Y} \subseteq \mathbb{R}$. Till now, we set the learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ in the linear regression with hypothesis class $\mathcal{H} = \{x \rightarrow \langle w, x \rangle : w \in \mathbb{R}^d\}$, loss $\ell(h, (x, y)) = (h(x) - y)^2$, and examples domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ with $\mathcal{X} \in \mathbb{R}^d$ and $\mathcal{Y} \in \mathbb{R}$. Because learning problem involves only linear functions as predictors

$h(x) = \langle w, x \rangle$, this learning problem could be defined equivalently with a hypothesis class $\mathcal{H} = \{w \in \mathbb{R}^d\}$ and loss function $\ell(w, (x, y)) = (\langle w, x \rangle - y)^2$. The latter will be mainly used.

APPENDIX A. USEFUL BITS

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 $x \in \mathbb{R}^d$ and $f : \mathbb{R}^d \rightarrow \mathbb{R}$ then

$$\begin{cases} f(E(x)) \leq E(f(x)) & \text{if } f \text{ is convex} \\ f(E(x)) \geq E(f(x)) & \text{if } f \text{ is concave} \end{cases}$$

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

Handout 1: 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:

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

1. MOTIVATIONS

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

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

Note 3. To overcome this problem, we will introduce the concept of surrogate loss function that allows a non-convex problem to be handled with the tools introduced in the convex setting.

2. CONVEX LEARNING PROBLEMS

Definition 4. Convex learning problem is a learning problem $(\mathcal{H}, \mathcal{Z}, \ell)$ that the hypothesis class \mathcal{H} is a convex set, and the loss function ℓ is a convex function for each example $z \in \mathcal{Z}$.

Example 5. Multiple linear regression $\langle w, x \rangle \rightarrow y$ with $y \in \mathbb{R}$, hypothesis class $\mathcal{H} = \{w \in \mathbb{R}^d\}$ and loss $\ell(w, (x, y)) = (\langle w, x \rangle - y)^2$ with

$$w^* = \arg \min_{\forall w} \mathbb{E} (\langle w, x \rangle - y)^2$$

or

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

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

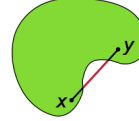
3. CONVEXITY

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

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



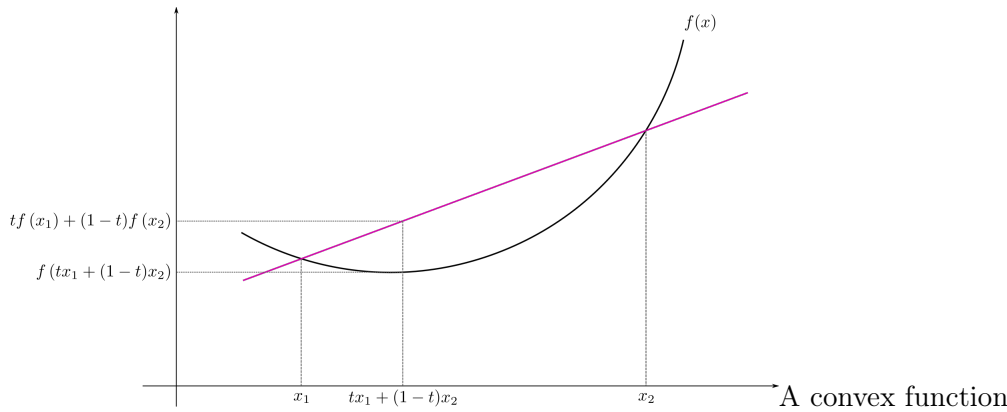
A convex set



A non-convex set

Definition 7. Let C be a convex set. A function $f : C \rightarrow \mathbb{R}$ is convex function if for any $u, v \in C$ and for any $\alpha \in [0, 1]$

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



A convex function

Example 8. The function $f : \mathbb{R} \rightarrow \mathbb{R}_+$ with $f(x) = x^2$ is convex function. For any $u, v \in C$ and for any $\alpha \in [0, 1]$ it is

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

Proposition 9. Every local minimum of a convex function is the global minimum.

Proposition 10. Let $f : C \rightarrow \mathbb{R}$ be convex function. The tangent of f at $w \in C$ is below f , namely

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

Proposition 11. Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $f(w) = g(\langle w, x \rangle + y)$ for some $x \in \mathbb{R}^d$, $y \in \mathbb{R}$. If g is convex function then f is convex function.

Proof. See Exercise 1 in the Exercise sheet. □

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

Example 13. Let $f_j : \mathbb{R}^d \rightarrow \mathbb{R}$ convex functions for $j = 1, \dots, r$. Then:

- (1) $g(x) = \max_{j=1, \dots, r} (f_j(x))$ is a convex function
- (2) $g(x) = \sum_{j=1}^r w_j f_j(x)$ is a convex function where $w_j > 0$

Solution.

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

$$\begin{aligned}
 g(\alpha u + (1 - \alpha)v) &= \max_{\forall j} (f_j(\alpha u + (1 - \alpha)v)) \\
 &\leq \max_{\forall j} (\alpha f_j(u) + (1 - \alpha)f_j(v)) && (f_j \text{ is convex}) \\
 &\leq \alpha \max_{\forall j} (f_j(u)) + (1 - \alpha) \max_{\forall j} (f_j(v)) && (\max(\cdot) \text{ is convex}) \\
 &\leq \alpha g(u) + (1 - \alpha)g(v)
 \end{aligned}$$

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

$$\begin{aligned}
 g(\alpha u + (1 - \alpha)v) &= \sum_{j=1}^r w_j f_j(\alpha u + (1 - \alpha)v) \\
 &\leq \alpha \sum_{j=1}^r w_j f_j(u) + (1 - \alpha) \sum_{j=1}^r w_j f_j(v) && (f_j \text{ is convex}) \\
 &\leq \alpha g(u) + (1 - \alpha)g(v)
 \end{aligned}$$

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

4. LIPSCHITZBNESS

Definition 15. Let $C \in \mathbb{R}^d$. Function $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$ is ρ -Lipschitz over C if for every $w_1, w_2 \in C$ we have that

$$(4.1) \quad \|f(w_1) - f(w_2)\| \leq \rho \|w_1 - w_2\|. \quad \text{Lipschitz condition}$$

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

Example 17. Consider the function $f : \mathbb{R} \rightarrow \mathbb{R}_+$ with $f(x) = x^2$.

(1) f is not a ρ -Lipschitz in \mathbb{R} .

(2) f is a ρ -Lipschitz in $C = \{x \in \mathbb{R} : |x| < \rho/2\}$.

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

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

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

Theorem 18. Let functions g_1 be ρ_1 -Lipschitz and g_2 be ρ_2 -Lipschitz. Then f with $f(x) = g_1(g_2(x))$ is $\rho_1\rho_2$ -Lipschitz.

Solution. See Exercise 2 from the exercise sheet

Example 19. Let functions g be ρ -Lipschitz. Then f with $f(x) = g(\langle v, x \rangle + b)$ is $(\rho \|v\|)$ -Lipschitz.

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

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

5. SMOOTHNESS

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

$$(5.1) \quad \|\nabla f(w_1) - \nabla f(w_2)\| \leq \beta \|w_1 - w_2\|.$$

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

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

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

$$f(v) \geq f(w) + \langle \nabla f(w), v - w \rangle$$

holds. Hence if both conditions imply upper and lower bounds

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

Remark 24. If $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is β -smooth then for $v, w \in \mathbb{R}^d$ such that $v = w - \frac{1}{\beta} \nabla f(w)$ then by (5.2), it is

$$\frac{1}{2\beta} \|\nabla f(w)\|^2 \leq f(w) - f(v)$$

If additionally $f(x) > 0$ for all $x \in \mathbb{R}^d$ then

$$\|\nabla f(w)\|^2 \leq 2\beta f(w)$$

which provides assumptions to bound the gradient.

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

Solution. See Exercise 3 from the Exercise sheet

Example 26. Let $f(w) = (\langle w, x \rangle + y)^2$ for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. Then f is $(2\|x\|^2)$ -smooth.

Solution. It is $f(w) = g(\langle w, x \rangle + y)$ for $g(a) = a^2$. g is 2-smooth since

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

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

6. NON-CONVEX LEARNING PROBLEMS (SURROGATE TREATMENT)

Remark 27. A learning problem may involve non-convex loss function $\ell(w, z)$ which implies a non-convex risk function $R_g(w)$. However, our learning algorithm will be analyzed in the convex setting. A suitable treatment to overcome this difficulty would be to upper bound the non-convex loss function $\ell(w, z)$ by a convex surrogate loss function $\tilde{\ell}(w, z)$ for all w , and use $\tilde{\ell}(w, z)$ instead of $\ell(w, z)$.

Example 28. Consider the binary classification problem with inputs $x \in \mathcal{X}$, outputs $y \in \{-1, +1\}$; we need to learn $w \in \mathcal{H}$ from hypothesis class $\mathcal{H} \subset \mathbb{R}^d$ with respect to the loss

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

with $y \in \mathbb{R}$, and $x \in \mathbb{R}^d$. Here $\ell(\cdot)$ is non-convex. A convex surrogate loss function can be

$$\tilde{\ell}(w, (x, y)) = \max(0, 1 - y\langle w, x \rangle)$$

which is convex (Example 14) wrt w . Note that:

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

Then we can compute

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

instead of

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

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 29. (Intuitions...) Using a convex surrogate loss function instead the convex one, facilitates computations but introduces extra error to the solution. If $R_g(\cdot)$ is the risk under the non-convex loss, $\tilde{R}_g(\cdot)$ is the risk under the convex surrogate loss, and \tilde{w}_{alg} is the output of the learning algorithm under $\tilde{R}_g(\cdot)$ then we have the upper bound

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

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.

Handout 0: Learning problem: Definitions, notation, and formulation –A recap

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

1. 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) is called the procedure where the ML model is tuned. **Training data** (or observations, sample data set, exemplars) is a set of observables $\{z_i \in \mathcal{Z}\}$ used to tune the parameters of the ML model. **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 focus here) and the unsupervised learning.

Supervised learning problems involve applications where the training data $z \in \mathcal{Z}$ comprises examples of the input vectors $x \in \mathcal{X}$ along with their corresponding target vectors $y \in \mathcal{Y}$; i.e. $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. **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 recover 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. $x \mapsto y$. Hence, \mathcal{X} is the input domain, and \mathcal{Y} is the output domain. The goal of learning is to discover a function which predicts $y \in \mathcal{Y}$ from $x \in \mathcal{X}$.

Unsupervised learning problems involve applications where the training data $z \in \mathcal{Z}$ consists 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 IN LEARNING

Definition 1. The learner's output is a function, $h : \mathcal{X} \rightarrow \mathcal{Y}$ 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. $h \in \mathcal{H}$.

Definition 3. Training data set \mathcal{S} of size m is any finite sequence of pairs $((x_i, y_i) ; i = 1, \dots, m)$ in $\mathcal{X} \times \mathcal{Y}$. This is the information that the learner has assess.

Definition 4. 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.

Definition 5. We denote as $\mathfrak{A}(\mathcal{S})$ the hypothesis (outcome) that a learning algorithm \mathfrak{A} returns given training sample \mathcal{S} .

Definition 6. (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 $\ell : \mathcal{H} \times \mathcal{Z} \rightarrow \mathbb{R}_+$. The purpose of loss function $\ell(h, z)$ is to quantify the “error” for a given hypothesis h and example z –the greater the error the greater its value of the loss.

Example 7. In binary classification problems where $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ and $\mathcal{Y} = \{0, 1\}$ is discrete, a loss function can be

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

Example 8. In regression problems $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ and \mathcal{Y} is uncountable, a loss function can be

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

Definition 9. (Risk function) The risk function $R_g(h)$ of h is the expected loss of the hypothesis $h \in \mathcal{H}$, w.r.t. probability distribution g over domain \mathcal{Z} ; i.e.

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

Remark 10. In learning, an ideal way to obtain an optimal predictor h^* is to compute the risk minimizer

$$h^* = \arg \min_{\mathcal{H}} (R_g(h))$$

Example 11. (Cont. Ex. 8) The risk function is $R_g(h) = \mathbb{E}_{z \sim g} (h(x) - y)^2$, and it measures the quality of the hypothesis function $h : \mathcal{X} \rightarrow \mathcal{Y}$ as the expected square difference between the predicted values h and the true target values y at every x .

Remark 12. 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). Suboptimally, one may resort to the Empirical risk function.

Definition 13. (Empirical risk function) The empirical risk function $\hat{R}_S(h)$ of h is the expectation of loss of h over a given sample $S = (z_1, \dots, z_m) \in \mathcal{Z}^m$; i.e.

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

Example 14. (Cont. Example 11) Given given sample $S = \{(x_i, y_i); i = 1, \dots, m\}$ the empirical risk function is $\hat{R}_S(h) = \frac{1}{m} \sum_{i=1}^m (h(x_i) - y_i)^2$.

Example 15. 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 $f(y|\theta)$ where the parameter θ is unknown. 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

$$(2.2) \quad R_g(\theta) = \mathbb{E}_{z \sim g} \left(\log \left(\frac{g(z)}{f_\theta(z)} \right) \right) = \mathbb{E}_{z \sim g} (\log(g(z))) - \mathbb{E}_{z \sim g} (\log(f_\theta(z)))$$

whose minimizer is

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

as the first term in (2.2) is constant. Note that in the Maximum Likelihood Estimation technique the MLE θ_{MLE} is the minimizer of

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

where $S = \{y_1, \dots, y_m\}$ is an IID sample from g . Hence, MLE θ_{MLE} can be considered as the minimizer of the empirical risk $R_S(\theta) = \frac{1}{m} \sum_{i=1}^m (-\log(f_\theta(z_i)))$.

Example 16. (Linear Regression) Consider the multiple linear regression problem $x \mapsto y$ where $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and $y \in \mathcal{Y} \subseteq \mathbb{R}^d$.

- The hypothesis is a linear function $h : \mathcal{X} \rightarrow \mathcal{Y}$ (that learner wishes to learn) to approximate mapping $x \mapsto y$. The hypothesis set $\mathcal{H} = \{ \langle w, x \rangle \mapsto y : w \in \mathbb{R}^d \}$. We can use the loss $\ell(h, (x, y)) = (h(x) - y)^2$.
- Equivalently, learning problem can be set differently because the predictor (linear function) is parametrized by $w \in \mathbb{R}^d$ as $\langle w, x \rangle \mapsto y$. Set $\mathcal{H} = \{w \in \mathbb{R}^d\}$. The set of examples is $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. The loss is $\ell(w, (x, y)) = (\langle w, x \rangle - y)^2$.

Handout 2: 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:

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

1. MOTIVATIONS

Note 1. 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 $\{z_i; i = 1, \dots, n\}$ generated from the data generating model $g(\cdot)$ and using loss $\ell(\cdot)$; that is

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

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

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

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

where here $f : \mathbb{R}^d \rightarrow \mathbb{R}$, 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 $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is a differentiable function.

Definition 4. Given a per-specified learning rate $\eta_t > 0$, the Gradient Descent (GD) algorithm for the solution of the minimization problem (2.1) is given in Algorithm 1

Algorithm 1 Gradient descent algorithm with learning rate η_t

For $t = 1, 2, 3, \dots$ iterate:

(1) compute

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

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

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

where

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

is the gradient of f at w .

Remark 5. Interpreting GD, GD produces a chain $\{w^{(t)}\}$ that drifts towards the 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 .

Remark 6. For more intuitive explanation, 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

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

See
Handout 1

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 $w^{(t)}$

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

while hoping that this mechanism would push the produced chain $\{w^{(t)}\}$ 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

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

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

Remark 7. Given T GD algorithm iterations, 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)

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

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

Remark 9. The parameter η_t is called learning rate, step size, or 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 8) 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 $\lim_{t \rightarrow \infty} \eta_t = 0$. 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 $\lim_{t \rightarrow \infty} \eta_t = \tau_*$ 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 $t \leq T_0$) 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 ($t \leq T_0$) is called burn-in; the values $\{w_t\}$ produced during the burn-in ($t \leq T_0$) are often discarded/ignored from the output of the GD algorithm.

- Parameters $C, \varsigma, \tau_*, T_0$ may be chosen based on pilot runs.

Remark 10. There are several practical termination criteria that can be used in GD Algorithm 1(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 $\|\nabla f(w^{(t)})\| \leq \epsilon$ for some pre-specified tiny $\epsilon > 0$ then STOP
- (2) terminate when the chain $w^{(t)}$ does not change; i.e. if $\|w^{(t+1)} - w^{(t)}\| \leq \epsilon \|w^{(t)}\|$ 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 11. 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.

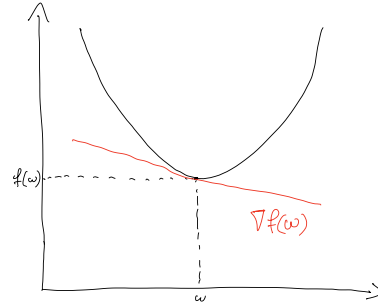
Definition 12. Vector v is called subgradient of a function $f : S \rightarrow \mathbb{R}$ at $w \in S$ if

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

Note 13. 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

Notation 14. The set of subgradients of function $f : S \rightarrow \mathbb{R}$ at $w \in S$ is denoted by $\partial f(w)$.

Definition 15. The Gradient Descent algorithm using subgradients in non-differentiable cases, results by replacing the gradient $\nabla f(w^{(t)})$ in (2.2) with any of subgradient v_t from the set of subgradients $\partial f(w^{(t)})$ at $w^{(t)}$; namely

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

3.1. Construction of subgradient.

Note 16. We discuss how to construct subgradients in practice.

Fact 17. *Some properties of subgradient sets that help for their construction*

- (1) *If function $f : S \rightarrow \mathbb{R}$ 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*

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

Example 18. Consider the function $f : \mathbb{R} \rightarrow \mathbb{R}_+$ 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 17, 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

Assumption 19. *For the sake of the analysis of the GD, let us consider:*

- (1) *constant learning rate $\eta_t = \eta$,*
- (2) *GD output $w_{GD}^{(T)} = \frac{1}{T} \sum_{t=1}^T w^{(t)}$*

Also as we will see, function $f(\cdot)$ should be convex and Lipschitz fin order for the following results to hold

Notation 20. w^* is the minimizer in (2.1).

Note 21. We consider Lemma 22 as given Fact.

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

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

Proof. Omitted; see the 2nd reference. \square

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

Proposition 24. *Consider the minimization problem (2.1). Given Assumptions 19, the error can be bounded as*

$$(4.2) \quad f(w_{\text{GD}}^{(T)}) - f(w^*) \leq \frac{1}{T} \sum_{t=1}^T \langle w^{(t)} - w^*, v_t \rangle$$

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

Proof. It is¹

$$(4.3) \quad \begin{aligned} f(w_{\text{GD}}^{(T)}) - f(w^*) &= f\left(\frac{1}{T} \sum_{t=1}^T w_t\right) - f(w^*) \\ &\leq \frac{1}{T} \sum_{t=1}^T (f(w_t) - f(w^*)) && \text{(by Jensen's inequality)} \\ &\leq \frac{1}{T} \sum_{t=1}^T \langle w^{(t)} - w^*, \nabla f(w^{(t)}) \rangle && \text{(by convexity of } f(\cdot) \text{)} \end{aligned}$$

\square

Note 25. The following provides conditions under which the gradient (or sub-gradient) is bounded. This is necessary in order to bound (4.2) with (4.1) in a meaningful manner.

Proposition 26. *$f : S \rightarrow \mathbb{R}$ 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. \implies Let $f : S \rightarrow \mathbb{R}$ 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

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

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

For \Leftarrow see Exercise 4 in the Exercise sheet. \square

¹Jensen's inequality for convex $f(\cdot)$ is $E(f(x)) \leq f(E(x))$

²If 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 $u \in S$

Note 27. The following summaries Lemma 22, and Propositions 24, 26 with respect to the GD algorithm.

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

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

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

Solution. Straightforward from Lemma 22, and Propositions 24, 26.

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 $w_{\text{GD}}^{(T)} = \frac{1}{T} \sum_{t=1}^T w^{(t)}$. Then*

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

$$(4.4) \quad f\left(w_{\text{GD}}^{(T)}\right) - f\left(w^*\right) \leq \frac{B\rho}{\sqrt{T}}$$

(2) *a given level off accuracy ε such that $f\left(w_{\text{GD}}^{(T)}\right) - f\left(w^*\right) \leq \varepsilon$ 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. \square

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).

Remark 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. EXAMPLES³

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

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

³Code is available in https://github.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2023/tree/main/Lecture_handouts/code/02.Gradient_descent/example_1.R

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

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

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

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

The GD Algorithm 1 with learning rate η is

For $t = 1, 2, 3, \dots$ iterate:

(1) compute

$$(5.3) \quad w^{(t+1)} = w^{(t)} - \eta v_t,$$

$$\text{where } v_t = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \bar{x} - 2\bar{y} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \bar{x}^2 - 2y^\top x \end{pmatrix}$$

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

If $t \geq T$ 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

$$\nabla \hat{R}_{\mathcal{D}}(w) = \begin{pmatrix} \frac{d}{dw_1} \hat{R}_{\mathcal{D}}(w) \\ \frac{d}{dw_2} \hat{R}_{\mathcal{D}}(w) \end{pmatrix} = \dots = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)} \bar{x} - 2\bar{y} \\ 2w_1^{(t)} \bar{x} + 2w_2^{(t)} \bar{x}^2 - 2y^\top x \end{pmatrix}$$

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 $\{(w^{(t)})\}$ and error $\hat{R}_{\mathcal{D}}(w^{(t)}) - \hat{R}_{\mathcal{D}}(w^*)$ 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 $\{(w^{(t)})\}$, and of the error $\hat{R}_{\mathcal{D}}(w^{(t)}) - \hat{R}_{\mathcal{D}}(w^*)$ 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 5.1a and 5.1b.



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



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



(C) $\hat{R}_D(w^{(t)}) - \hat{R}_D(w^*)$



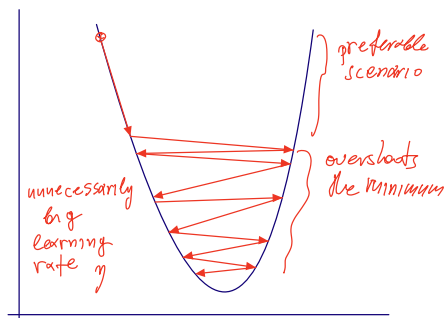
(D) $\{w_1^{(t)}\}$



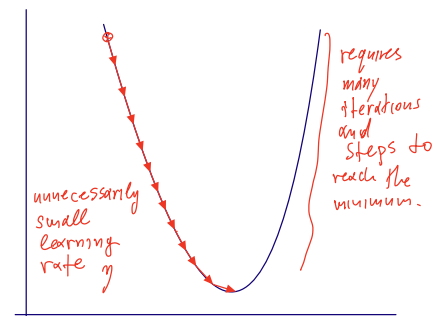
(E) $\{w_2^{(t)}\}$



(F) $\hat{R}_D(w^{(t)}) - \hat{R}_D(w^*)$



(A) Unnecessarily large learning rate



(B) Unnecessarily small learning rate

Handout 3: 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:

- Shalev-Shwartz, S., & Ben-David, S. (2014). Understanding machine learning: From theory to algorithms. Cambridge university press.
- Bottou, L. (2012). Stochastic gradient descent tricks. In Neural networks: Tricks of the trade (pp. 421-436). Springer, Berlin, Heidelberg.

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) $R(w) = \mathbb{E}_{z \sim g}(\ell(w, z))$ given an unknown data generating model $g(\cdot)$ and using a known tractable loss $\ell(\cdot, \cdot)$; that is

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

Remark 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).

Remark 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 ($n \approx \text{big}$). 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.

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

2. STOCHASTIC GRADIENT DESCENT

2.1. Description.

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

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

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

Algorithm 6. *Stochastic Gradient Descent (SGD) with learning rate $\eta_t > 0$ for the solution of the minimization problem (2.1)*

For $t = 1, 2, 3, \dots$ iterate:

(1) compute

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

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

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

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

Remark 7. If f is differentiable at $w^{(t)}$, it is $\partial f(w^{(t)}) = \{\nabla f(w^{(t)})\}$. Hence v_t is such as $\mathbb{E}(v_t | w^{(t)}) = \nabla f(w^{(t)})$ 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

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

where

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

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

Remark 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)

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

(2) or the best value discovered

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

(3) or the last value discovered

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

Note 10. SGD output converges to a local minimum, $w_{\text{SGD}}^{(T)} \rightarrow w_*$ (in some sense), under different sets of regularity conditions. Section 4 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) $\sum_{t=1}^{\infty} \eta_t^2 < \infty$

Remark 12. The popular learning rates $\{\eta_t\}$ in Remark 9 in Handout 2 satisfy Condition 11 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.

Remark 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 $t \rightarrow \infty$; if this was not the case then

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

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

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

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. STOCHASTIC GRADIENT DESCENT WITH PROJECTION

Remark 14. 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 $w_{\text{SGD}} \notin \mathcal{H}$. SGD can be modified to address this issue, as in Algorithm 15, by including a projection step guarantying $w \in \mathcal{H}$.

Algorithm 15. *Stochastic Gradient Descent with learning rate $\eta_t > 0$ and with projection in \mathcal{H} for problem in (2.1)*

For $t = 1, 2, 3, \dots$ iterate:

(1) compute

$$(3.1) \quad w^{(t+\frac{1}{2})} = w^{(t)} - \eta_t v_t,$$

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

(2) compute

$$(3.2) \quad w^{(t+1)} = \arg \min_{w \in \mathcal{H}} \left(\|w - w^{(t+\frac{1}{2})}\| \right)$$

(3) terminate if a termination criterion is satisfied

4. ANALYSIS OF SGD (ALGORITHM 6)

Note 16. Recall that the stochasticity of SGD comes from the stochastic sub-gradients $\{v_t\}_{t=1}^T$; hence the expectations below are under these random vectors' distributions.

Theorem 17. *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*

$$(4.1) \quad \mathbb{E} \left(f \left(w_{\text{GD}}^{(T)} \right) \right) - f(w^*) \leq \frac{\|w^*\|^2}{2\eta T} + \frac{\eta}{2} \frac{1}{T} \sum_{t=1}^T \mathbb{E} \|v_t\|^2$$

Proof. Let $v_{1:t} = (v_1, \dots, v_t)$. By Jensens' inequality (or see (4.3) in Handout 2)

$$(4.2) \quad \mathbb{E} \left(f \left(w_{\text{GD}}^{(T)} \right) - f(w^*) \right) \leq \mathbb{E} \left(\frac{1}{T} \sum_{t=1}^T \left(f(w^{(t)}) - f(w^*) \right) \right) = \frac{1}{T} \sum_{t=1}^T \mathbb{E} \left(f(w^{(t)}) - f(w^*) \right)$$

I will try to use Lemma 22 from Handout 2, hence I need to show

$$(4.3) \quad \mathbb{E} \left(f(w^{(t)}) - f(w^*) \right) \leq \mathbb{E} \left(\langle w^{(t)} - w^*, v_t \rangle \right)$$

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

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

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

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

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

$$(4.4) \quad \begin{aligned} \mathbb{E}_{v_{1:t-1}} \left(\langle w^{(t)} - w^*, \mathbb{E}_{v_{1:t}} (v_t | v_{1:t-1}) \rangle \right) &\geq \mathbb{E}_{v_{1:t-1}} \left(f(w^{(t)}) - f(w^*) \right) \\ &= \mathbb{E}_{v_{1:T}} \left(f(w^{(t)}) - f(w^*) \right) \end{aligned}$$

Hence combining (4.4), (4.3), and (4.2)

$$\mathbb{E} \left(f \left(w_{\text{GD}}^{(T)} \right) - f(w^*) \right) \leq \frac{1}{T} \sum_{t=1}^T \mathbb{E} \left(\langle w^{(t)} - w^*, v_t \rangle \right)$$

Then Lemma 22 in Handout 2 implies

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

□

Remark 18. The upper bound in (4.1) depends on the variation of v_t as

$$(4.5) \quad \mathbb{E} \|v_t\|^2 = \sum_{j=1}^d \text{Var}(v_{t,j}) + \sum_{j=1}^d (\mathbb{E}(v_{t,j}))^2$$

where d is the dimension of $v_t = (v_{t,1}, \dots, v_{t,d})^\top$. The second term on the right hand side of (4.5) is constant as $v_{t,j}$ is the unbiased estimator of the sub-gradient by construction.

Proposition 19. (*Cont. Theorem 17*) Let $f(\cdot)$ be a convex function, and let $\mathcal{H} = \{w \in \mathbb{R} : \|w\| \leq B\}$. Let $\mathbb{E} \|v_t\|^2 \leq \rho^2$. Assume we run SGD algorithm of $f(\cdot)$ with learning rate $\eta_t = \sqrt{\frac{B^2}{\rho^2 T}}$ for T steps, and output $w_{\text{SGD}}^{(T)} = \frac{1}{T} \sum_{t=1}^T w^{(t)}$. Then

(1) upper bound on the sub-optimality is

$$(4.6) \quad \mathbb{E} \left(f \left(w_{\text{SGD}}^{(T)} \right) \right) - f(w^*) \leq \frac{B\rho}{\sqrt{T}}$$

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

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

Proof. It follows from 17. □

Remark 20. Lemma 22 in Handout 2 holds even when projection steps are added in the vanilla SGD algorithm, hence the above analysis holds for the SGD with projections (Algorithm 15) too.

5. IMPLEMENTATION OF SGD IN THE LEARNING PROBLEM 1

Note 21. Below we show SGD can be implement in the learning Problem 1. Proposition 22 allows a convenient implementation of SGD to the learning problem (Problem 1).

Proposition 22. For a randomly drawn $z \sim g(\cdot)$, 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

$$(5.1) \quad \ell(u, z) - \ell(w, z) \geq \langle u - w, v \rangle$$

It is

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

Hence, by definition, v is such that $\mathbb{E}_{z \sim g} (v | w)$ 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

$$\mathbb{E}_{z \sim g} (v | w) = \nabla_w R_g(w)$$

Note 24. Below we show how SGD can be implement in the learning Problem 1.

Note 25. Assume there is available a finite dataset $\mathcal{S}_n = \{z_i; i = 1, \dots, n\}$ of size n which consists of independent realizations z_i from the data generating distribution g ; $z_i \stackrel{\text{ind}}{\sim} g$. Batch sampling (Algorithm 26) is an implementation of the SGD (Algorithm 6) in the learning Problem 1.

Algorithm 26. *batch Stochastic Gradient Descent with learning rate $\eta_t > 0$, and batch size m , for Problem 1.*

For $t = 1, 2, 3, \dots$ iterate:

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

(2) compute

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

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

(3) terminate if a termination criterion is satisfied

Remark 27. Step 1 can be presented equivalently as

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

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

Remark 28. A projection step, such as (3.2) can be added right after step 2 in Algorithm 26, if needed.

Remark 29. 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 26 can become

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

Definition 30. Online Stochastic gradient descent is the special case of Algorithm 26 using sub-samples of size one ($m = 1$), namely, only one example is randomly chosen in Step 1 of Algorithm 26.

Remark 31. In theory, using larger batch size m has the benefit that reduces the variance $\text{Var}(v_t | w^{(t)})$ of v_t at iteration t due to averaging effect, stabilizes the SGD algorithm, and reduces the error bound (4.1); see Remark 18.

Remark 32. 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 in a scenario with big-data: 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.

Remark 33. 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.

6. STOCHASTIC VARIANCE REDUCED GRADIENT (SVRG)

Remark 34. Recall the upper bound of the error (4.1) in SGD depends on the variance of the stochastic gradient, as shown in Remark 4.5. Hence the algorithm may be improved by reducing the variance of each element of v_t .

Remark 35. Control variate is a general way to perform variance reduction. Let random variables $v \in \mathbb{R}$, and $y \in \mathbb{R}$. Let $z = v + c(y - \mathbb{E}(y))$ for some constant $c \in \mathbb{R}$. It is $\mathbb{E}_c(z) = \mathbb{E}(v)$ and

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

which is minimized for

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

hence

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

Note 36. For simplicity, SVRG is presented in the case where $\kappa = 1$ and the loss function $\ell(w, z)$ is differentiable wrt w hence its gradient exists. However it is applicable to the more general cases introduced.

Remark 37. Every m iterations, SVRG keeps a snapshot \tilde{w} , and computes the gradient using all data i.e. $\frac{1}{n} \sum_{i=1}^n \ell(\tilde{w}, z_i)$. At each iteration t , the update is

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

given that a random $\tilde{z}^{(t)}$ has been collected from the sample. The symbols below the brackets are given with reference to Remark 35.

Algorithm 38. *Stochastic Variance Reduced Gradient with learning rate $\eta_t > 0$ for Problem 1.*

For $t = 1, 2, 3, \dots$ iterate:

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

(2) compute

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

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

(4) if a termination criterion is satisfied STOP

Remark 39. Iterations of SVRG are computationally faster than those of full GD, but SVRG can still match the theoretical convergence rate of GD.

Remark 40. How often we get snapshots, κ , in Algorithm 38 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.

7. PRECONDITIONED SGD; THE ADAGRAD ALGORITHM

Remark 41. 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 42. To address this, SGD (Algorithm 6) can be modified in the update step as in Algorithm 43 by using a preconditioner P_t that accounts for the curvature (or geometry in general of f).

Algorithm 43. *Preconditioned Stochastic Gradient Descent with learning rate $\eta_t > 0$, and preconditioner P_t for the solution of the minimization problem (2.1)*

For $t = 1, 2, 3, \dots$ iterate:

(1) compute

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

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

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

If $t \geq T$ then STOP

Remark 44. A natural choice of P_t can be $P_t := [H_t + \epsilon I_d]^{-1}$, where H_t is the Hessian matrix $[H_t]_{i,j} = \frac{\partial^2}{\partial w_i \partial w_j} f(w) \Big|_{w=w^{(t)}}$ (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 45. 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 46. AdaGrad dynamically incorporates knowledge of the geometry of function $f(\cdot)$ (to be minimized) in earlier iterations to perform more informative gradient-based learning.

Remark 47. 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 48. Hence, this strategy often improves convergence performance over standard stochastic gradient descent in settings where data is sparse and sparse features w 's are more informative.

Definition 49. Adaptive Stochastic Gradient Decent (AdaGrad) can be presented in terms of preconditioned SGD (Algorithm 43) with preconditioner $P_t = [I_d \text{diag}(G_t) I_d + \epsilon I_d]^{-1/2}$ in (7.1)

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

where $\text{diag}(A) := (A_{1,1}, A_{2,2}, \dots, A_{d,d})^\top$ is the vector of the diagonal of a matrix A , $G_t = \sum_{\tau=1}^t v_\tau^\top v_\tau$ 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 in case the gradient becomes too close to zero.

Remark 50. 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

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

where j denotes the j -th dimension of w . Hence (7.2) implies 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 51. 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.

8. EXAMPLE¹

Note 52. We continue Example in Section 5 in Handout 2. Recall, we considered a hypothesis space \mathcal{H} of linear functions $h : \mathbb{R}^2 \rightarrow \mathbb{R}$ with $h(w) = w_1 + w_2x$, $w = (w_1, w_2)^\top$, and $\ell(w, z = (x, y)^\top) = (y_i - w_1 - w_2x)^2$. Here we consider a big dataset $\mathcal{S}_n = \{z_1, \dots, z_n\}$ with $n = 10^6$ examples.

Example 53. The batch SGD algorithm (Algorithm 26) with learning rate η_t and batch size $m = 10$ is

- For $t = 1, 2, 3, \dots$ iterate:
 - (1) Randomly generate a set $\mathcal{J}^{(t)}$ by drawing $m = 10$ numbers from $\{1, \dots, n = 10^6\}$, and set $\tilde{\mathcal{S}}_m = \{z_i; i \in \mathcal{J}^{(t)}\}$
 - (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

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

In Figures 8.1a & 8.1d, 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 $\{w^{(t)}\}$.

Example 54. The SVRG with learning rate $\eta_t > 0$ and batch size $m = 1$ is

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

$$(8.1) \quad w^{(t+1)} = \begin{bmatrix} w_1^{(t)} \\ w_2^{(t)} \end{bmatrix} - \eta_t \left(\begin{bmatrix} 2(w_1^{(t)} - \tilde{w}_1^{(t)}) + 2w_2^{(t)} x_{j^*} \\ 2(w_2^{(t)} - \tilde{w}_2^{(t)}) \bar{x} + 2(w_2^{(t)} (x_{j^*})^2 - \tilde{w}_2^{(t)} (x_{j^*})^2) \end{bmatrix} + \nabla \hat{R}_{\mathcal{D}}(\tilde{w}) \right)$$

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

$$(8.2) \quad \frac{1}{n} \sum_{i=1}^n \ell(\tilde{w}, z_i) = \begin{pmatrix} 2\tilde{w}_1^{(t)} + 2\tilde{w}_2^{(t)} \bar{x} - 2\bar{y} \\ 2\tilde{w}_1^{(t)} \bar{x} + 2\tilde{w}_2^{(t)} \bar{x}^2 - 2\bar{y}^\top \bar{x} \end{pmatrix} = \nabla \hat{R}_{\mathcal{D}}(\tilde{w})$$

- (4) if a termination criterion is satisfied STOP

¹Code can be found in https://github.com/georgios-stats/Machine_Learning_and_Neural_Networks_III_Epiphany_2023/tree/main/Lecture_handouts/code/03.Stochastic_gradient_descent

Because (8.2) is actually the gradient of the Risk function at \tilde{w} and

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

In Figure 8.1c we observe the frequency of the snapshots has improved the convergence; however this is not a panacea as seen in Figure 8.1f.

Example 55. The AdaGrad with $\eta_t = 1$, $\epsilon = 10^{-6}$, and batch size $m = 1$ is

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

$$v_t = \begin{pmatrix} 2w_1^{(t)} + 2w_2^{(t)}x_{j^*} - 2y_{j^*} \\ 2w_1^{(t)}\bar{x} + 2w_2^{(t)}x_{j^*}^2 - 2y_{j^*}x_{j^*} \end{pmatrix}$$

$$G_t = G_{t-1} + \begin{pmatrix} v_{t,1}^2 \\ v_{t,2}^2 \end{pmatrix}$$

$$w^{(t+1)} = \begin{pmatrix} w_1^{(t)} - \frac{\eta_t}{\sqrt{G_{t,1} + \epsilon}}v_{t,1} \\ w_2^{(t)} - \frac{\eta_t}{\sqrt{G_{t,2} + \epsilon}}v_{t,2} \end{pmatrix},$$

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

because

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

In Figures 8.1g & 8.1h, 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.

Example 56. Consider a (rather naive) loss function $\ell(w, z = (x, y)) = -\cos(0.5(y - w_1 - w_2x))$, a hypothesis class $\mathcal{H} = \{w \in \mathbb{R}^2 : \|w\| \leq 1.5\}$, 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 $t = 1, 2, 3, \dots$ iterate:
 - (1) randomly generate a set $\mathcal{J}^{(t)} = \{j^*\}$ by drawing one number from $\{1, \dots, n = 10^6\}$, and set $\tilde{\mathcal{S}}_1 = \{z_{j^*}\}$

(2) compute

$$w^{(t+1/2)} = w^{(t)} - \frac{50}{t} \begin{pmatrix} \sin(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}) \\ \sin(y_{j^*} - w_1^{(t)} - w_2^{(t)} x_{j^*}) x_{j^*} \end{pmatrix}$$

$$w^{(t+1/2)} = \arg \min_{\forall w: \|w\| \leq 1.5} (\|w - w^{(t+1/2)}\|)$$

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

because

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

In Figures 8.1b & 8.1e, 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.



(A) batch SGD Example 53 w_1



(B) online SGD with projection Example 56 w_1



(C) SVRG Example 54 w_1



(D) batch SGD Example 53 w_2



(E) online SGD with projection Example 56 w_2



(F) SVRG Example 54 w_2



(G) online AdaGrad Example 55 w_1



(H) online AdaGrad Example 55 w_2

FIGURE 8.1. Simulations of the Examples

Draft Handout 4: 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).

Reading list & references:

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

1. BAYESIAN LEARNING AND MOTIVATIONS

Remark 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 $\mathcal{S}_n = \{z_i; i = 1, \dots, n\}$ 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

$$(1.1) \quad \begin{cases} z_i|w & \stackrel{\text{ind}}{\sim} f(z_i|w), \text{ for } i = 1, \dots, n \\ w & \sim f(w) \end{cases}$$

Remark 3. Bayesian learning (inference) relies on the posterior distribution density

$$(1.2) \quad f(w|z_{1:n}) = \frac{L_n(w) f(w)}{\int L_n(w) f(w) dw}$$

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)

Remark 4. 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

$$(1.3) \quad \mathbb{E}_f(h(w) | z_{1:n}) = \int h(w) f(w | z_{1:n}) dw$$

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

Remark 5. 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.

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

$$(1.5) \quad = \arg \min_{w \in \Theta} \left(\underbrace{-\log(L_n(w))}_{(I)} - \underbrace{\log(f(w))}_{(II)} \right)$$

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

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

Remark 8. GD is particularly suitable to solve (2.1) when w has high dimensionality.

Algorithm 9. Gradient descent (Algorithm 1 Handout 2) with learning rate $\eta_t \geq 0$ can be used to solve (2.1) by using the update rule as

For $t = 1, 2, 3, \dots$ iterate:

(1) Compute

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

Remark 10. The implementation of other GD variants (eg (3.2) in Handout 2) is straightforward, based on Algorithm 9.

Remark 11. 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 32 and 33 of Handout 3.

Algorithm 12. *Batch Stochastic Gradient Descent (Algorithm 26 in Handout 3) with learning rate $\eta_t \geq 0$ and batch size m can be used to solve (2.1) by using the update rule as*

For $t = 1, 2, 3, \dots$ iterate:

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

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

Remark 13. Recursion (2.3) is justified in terms of SGD theory as

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

Remark 14. The implementation of the SGD variants (Algorithms 26, 38, 43, 49 in Handout 3) is straightforward based on Algorithm 12 and (2.4).

3. FULL BAYESIAN LEARNING VIA SGLD

Problem 15. 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

$$(1.3) \quad \mathbb{E}_f(h(w) | z_{1:n}) = \int h(w) f(w | z_{1:n}) dw$$

Remark 16. Monte Carlo integration aims at approximating (1.3), by using Central Limit Theorem or Law of Large Numbers arguments as $\hat{h} \approx \mathbb{E}_f(h(w) | z_{1:n})$ where

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

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

Remark 17. 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 16).

Remark 18. 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 16).

Note 19. 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 $\{w^{(t+1)}\}$ converges to samples that could have been drawn from the true posterior distribution.

Algorithm 20. *Stochastic Gradient Langevin Dynamics (SGLD) with learning rate $\eta_t > 0$, batch size m , and temperature $\tau > 0$ is*

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

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

where $\epsilon_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$.

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

Remark 21. The first few iterations from Algorithm 20 because they 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.

Remark 22. The output of SGLD (Algorithm 20) $\{w^{(t)}\}$ includes the generated values of w produced during the last few iterations of the running algorithm (aka the tail of the generated chain).

Remark 23. SGLD (Algorithm 20) generates as output a random chain $\{w^{(t)}\}$ that is approximately distributed according to a distribution with density such as

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

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

under regularity conditions. Conditions 11 on the learning rate are rather inevitable and should be satisfied.

Condition 24. 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) $\sum_{t=1}^{\infty} \eta_t^2 < \infty$

Remark 25. 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.

Remark 26. SGLD for $\tau = 1$ approximately simulates from the posterior (1.2).

Remark 27. The popular learning rates $\{\eta_t\}$ in Remark 9 in Handout 2 satisfy Condition 11 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.

Remark 28. (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

$$(3.5) \quad dW(t) = -\nabla_w [-\log f(W(t) | z_{1:n})] dt + \sqrt{2\tau} dB(t), \quad t \geq 0$$

where $\{B(t)\}$ is a standard Brownian motion¹ in \mathbb{R}^d (i.e.). Under suitable assumptions on f , it can be shown that a Gibbs distribution with PDF such as

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

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

Remark 29. (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 9 -but this is until η_t or $\nabla \log(L_n(w))$ 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 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.

Remark 30. 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 .

Remark 31. 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.

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

Remark 32. Expectation (1.3), can be estimated as an arithmetic average

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

as by LLN $\widehat{h_T(w)} \rightarrow E_f(h(w) | z_{1:n})$

Remark 33. Another more efficient estimator for the expectation (1.3) is the weighted arithmetic average

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

Because the step size decreases, the mixing rate of the chain $\{w^{(t)}\}$ 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.

Remark 34. 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. Hence the update (3.2) becomes

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

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

4. EXAMPLES ²

We continue the Example 33 in Handout 1, and Example 8 in Handout 2. Consider the Bayesian Normal linear regression model

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

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

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

Because SGD (Algorithm 12) and SGLD (Algorithm 20) can better handle cases when $w \in \mathbb{R}^d$, instead of $w = (\beta, \sigma^2) \in \mathbb{R}^d \times \mathbb{R}_+$, we consider a transformation $w = (\beta, \gamma) \in \mathbb{R}^d \times \mathbb{R}$ with

²Code 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

$\gamma = \log(\sigma^2)$. Hence, the Bayesian model becomes

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

where

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

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

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

Hence for the log sampling PDF I have

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

...so

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

Hence for the log a priori PDF I have

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

...so

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

After running SGD (Algorithm 12) and SGLD (Algorithm 20) with the computed gradients (4.1) and (4.2) for $w = (\beta, \gamma) \in \mathbb{R}^d \times \mathbb{R}$ with $\gamma = \log(\sigma^2)$, and obtaining chains $\{w^{(t)} = (\beta^{(t)}, \gamma^{(t)})\}_{t=1}^T$, if we are interested in learning (β, σ^2) we can just perform transformation $\{(\sigma^{(t)})^2 = \exp(\gamma^{(t)})\}_{t=1}^T$.

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

- In Figures 4.1, we ran the SGD for different batch sizes and compared it against the exact MLE. We observe that SGD trace converges to the exact MLE. The oscillation are due to the stochastic gradient (ie, noise in the gradient).
- In Figures 4.2, we ran the SGLD for different batch sizes m and compared it against the exact posterior densities. We observe that the histograms of $\{w^{(t)}\}$ produced from SGLD are closer to the curves representing the exact posteriors when the batch size is bigger. As we said this is not a panacea; if the landscape of the exact posterior 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 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 $\tau = 1$.

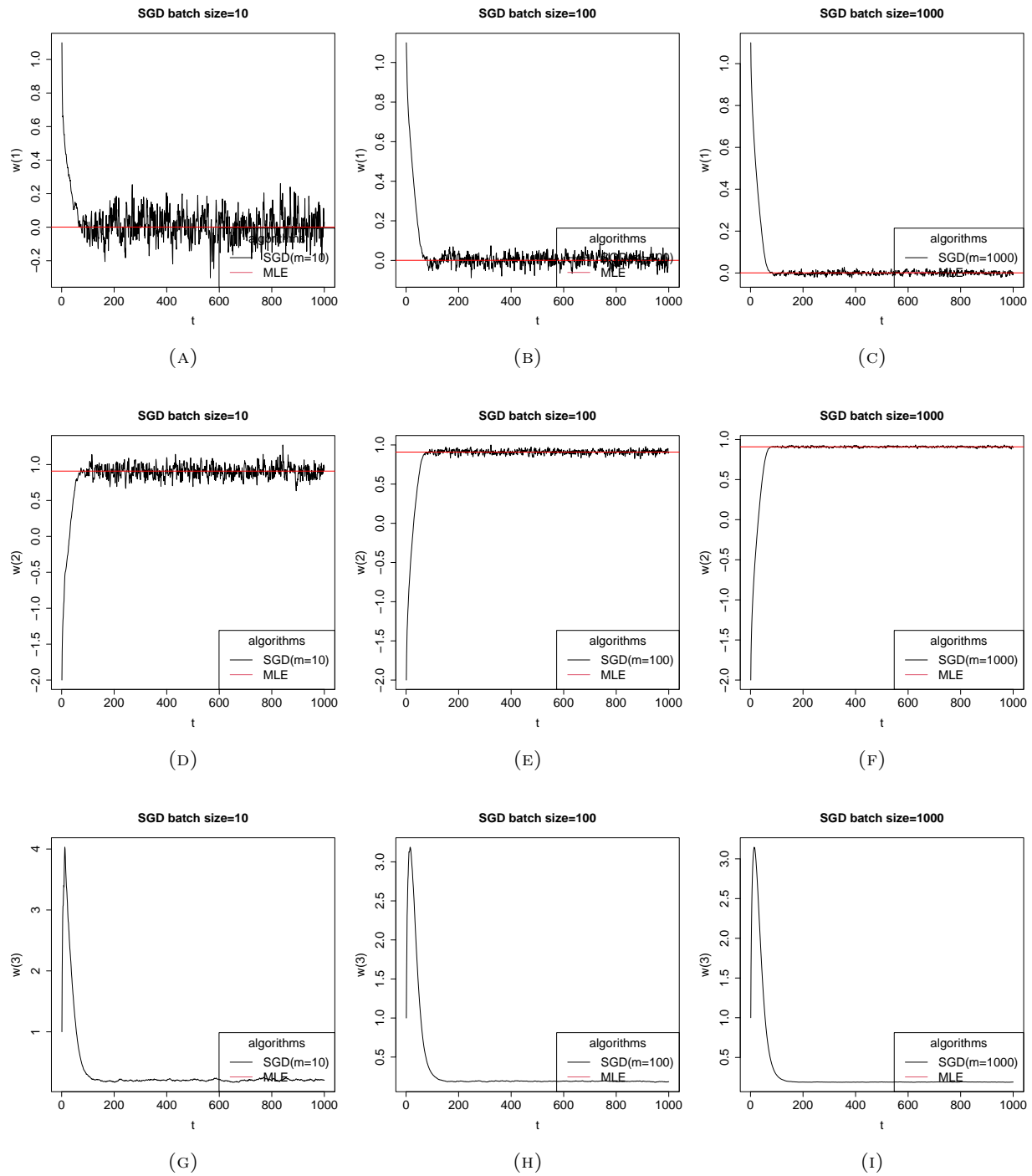


FIGURE 4.1. Bayesian learning via SGD (SGD vs (exact)MLE) Study on batch size m .

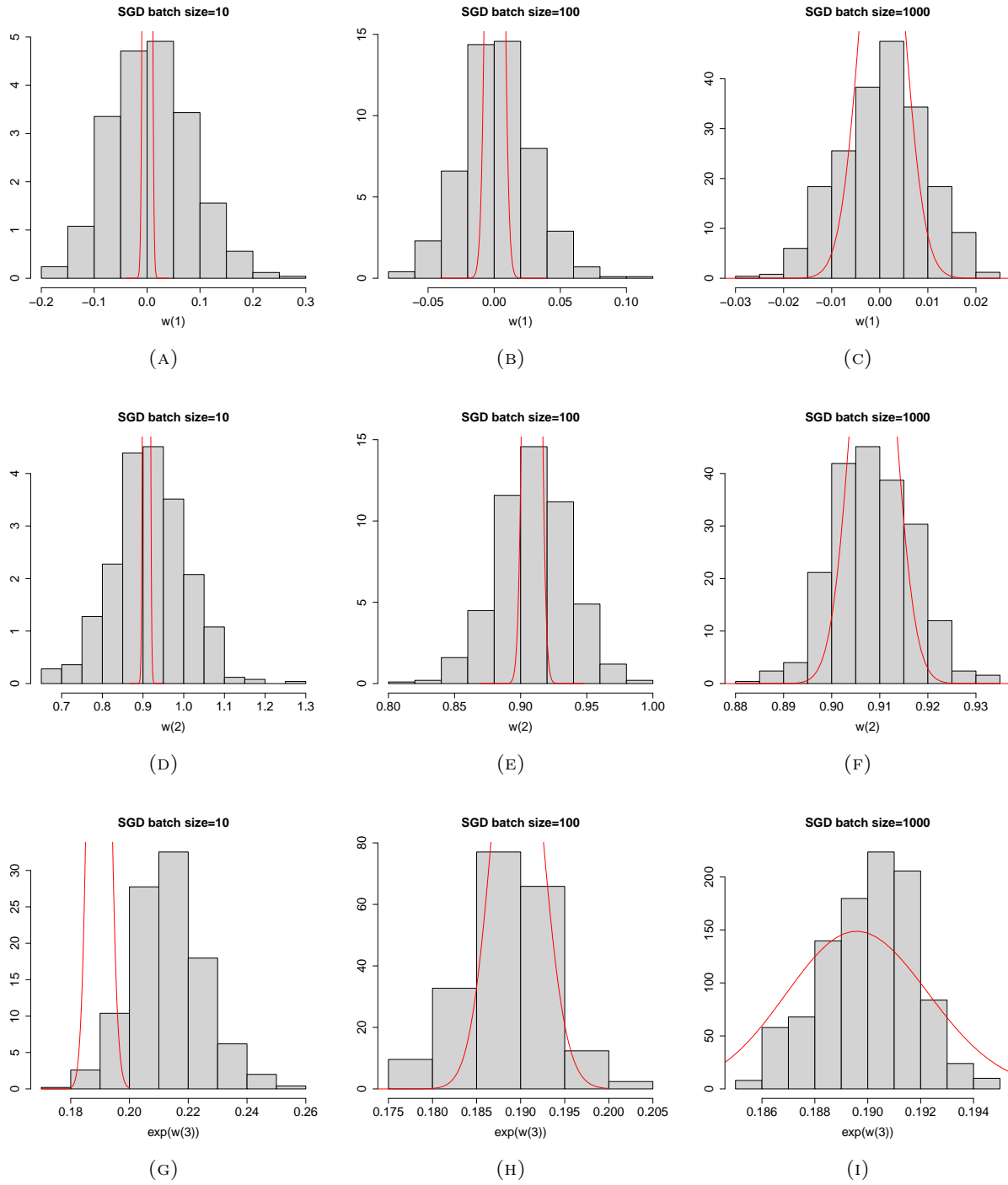


FIGURE 4.2. Bayesian learning: SGLD vs exact posterior (in red). Temperature $\tau = 1$. Study on batch size m

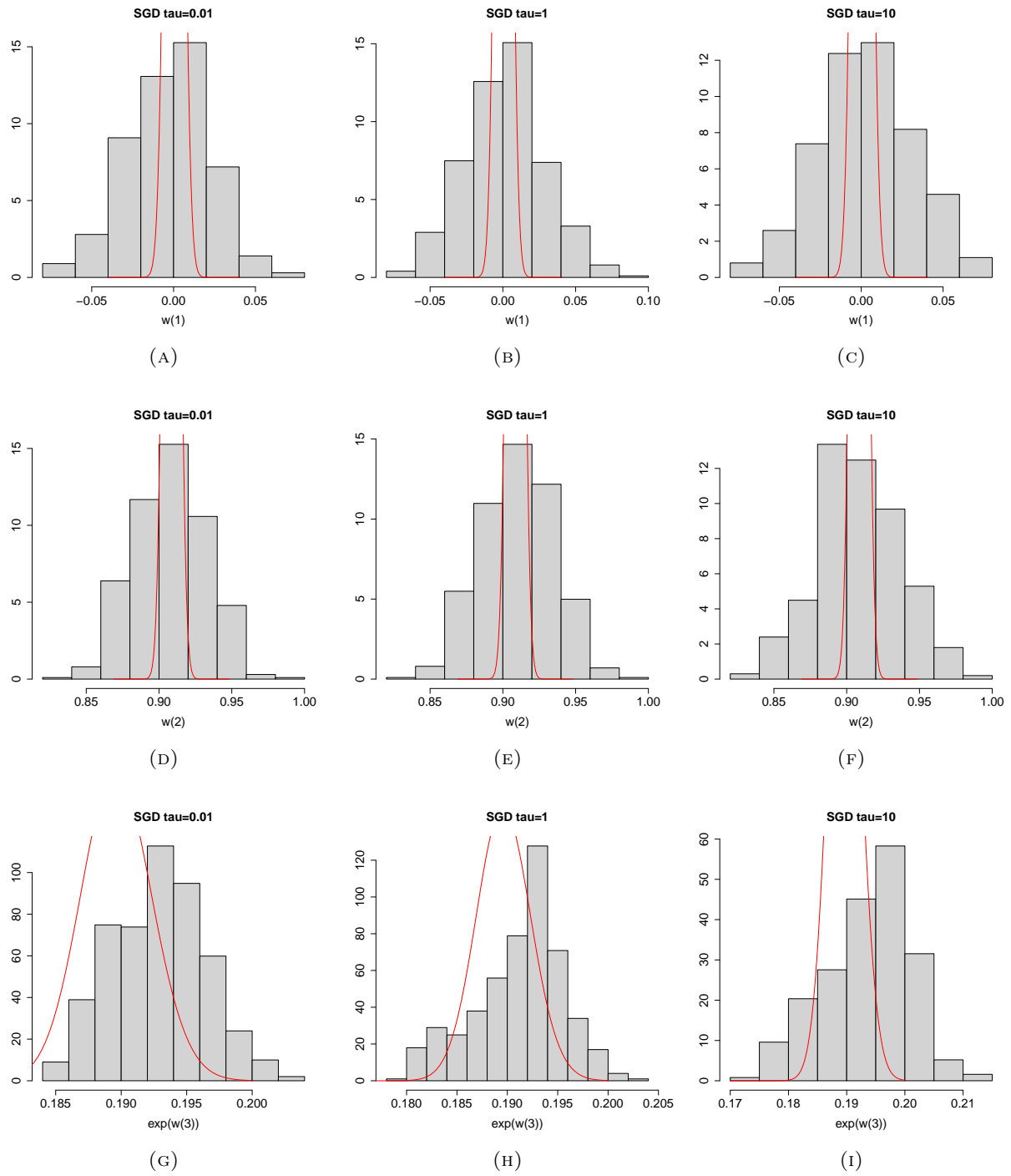


FIGURE 4.3. Bayesian learning: SGLD vs exact posterior (in red). Batch size = 100. Study on τ