Statistical Machine Learning - Seminar Notes

Tsinghua MSE

July 5, 2022

Contents

This note **aggregates** the contents from the following books, articles and notes:

- Bach 2021
- Mohri, Rostamizadeh, and Talwalkar 2018
- Shalev-Shwartz and Ben-David 2014
- Tropp 2012
- Wainwright 2019
- the lecture notes of Patrick Rebeschini

1 Introduction to Supervised Learning

1.1 Decision Theory

Main Concern. What is the optimal perforamce, regardless of the finiteness of the training data? In other words, if we have a perfect knowledge of the underlying probability distribution of the data, what should be done?

We consider a fixed (testing) distribution $P_{X,Y}(x, y)$ on $\mathcal{X} \times \mathcal{Y}$, with marginal distribution $P_X(x)$ on $\mathcal{X}$. At this point we make no assumptions on the input space $\mathcal{X}$.

1.1.1 Loss Functions

We consdier a loss function $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, where $l(y, \hat{y})$ is the loss of predicting $\hat{y}$ while the true label is y. Hera are some examples:

- **Binary classification**. $\mathcal{Y} = \{0, 1\}$ or $\mathcal{Y} = \{-1, 1\}$, and we consider the 0-1 loss

$$l(y, \hat{y}) = \mathbb{1}(y \neq \hat{y})$$

- **Multi-category classification**. $\mathcal{Y} = \{1, \ldots, k\}$ and still the 0-1 loss
- **Regression**. $\mathcal{Y} = \mathbb{R}$ and consider the square loss

$$l(y, \hat{y}) = (y - \hat{y})^2$$

or the abosulte loss

$$l(y, \hat{y}) = |y - \hat{y}|$$

which is often used for ”robust” estimamtion since the penaly for lager errors is smaller.

1.1.2 Risks

What should be the performance criterion for supervised learning? The answer is, given the loss function $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, we can define the expected risk or testing error of a function $f : \mathcal{X} \to \mathcal{Y}$ as the expectation of the loss function between the output y and the prediction $f(x)$.

Definition 1.1 (Expected Risk)**.** Given a loss function $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, and a distribution $P(x, y)$, the expected risk of a prediction function $f : \mathcal{X} \to \mathcal{Y}$ is defined as:

$$\mathcal{R}(f) = \mathbb{E}_{X,Y}\left[l(Y, f(X))\right] = \int_{\mathcal{X}\times\mathcal{Y}} l(y, f(x))dP(x, y) \tag{1.1}$$

Note that the risk depends on the joint distribution $P(x, y)$.

Definition 1.2 (Empirical Risk)**.** Given a loss function $l : \mathcal{Y}\times\mathcal{Y} \to \mathbb{R}$, and data $(x_i, y_i) \in \mathcal{X}\times\mathcal{Y}, i = 1, \ldots, n$, the empirical risk (training error) of a prediction function $f : \mathcal{X} \to \mathcal{Y}$ is defined as:

$$\hat{\mathcal{R}}(f) = \frac{1}{n}\sum_{i=1}^{n} l(y_i, f(x_i)) \tag{1.2}$$

where here $1/n$ is the empirical distribution function $\hat{P}(x, y)$.

- **Binary classification**. $\mathcal{Y} = \{0, 1\}$ and 0-1 loss $l(y, \hat{y}) = \mathbb{1}(y \neq \hat{y})$, we can express the risk as

$$\mathcal{R}(f) = \mathbb{E}_{X,Y}\big[\mathbb{1}(Y \neq f(X))\big] = \mathbb{P}(Y \neq f(X))$$

  which is simply the probability of making a mistake on the testing data; while the empricial risk is the proportion of mistake on tranining data

$$\hat{\mathcal{R}}(f) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}(y_i \neq f(x_i))$$

- **Multi-category classification**. $\mathcal{Y} = \{1, \dots, k\}$ and 0-1 loss, we can express the risk $\mathcal{R}(f)$ and empirical risk $\hat{\mathcal{R}}(f)$ in a similiar way.

- **Regression**. $\mathcal{Y} = \mathbb{R}$ and the square loss $l(y, \hat{y}) = (y - \hat{y})^2$, the risk is then

$$\mathcal{R}(f) = \mathbb{E}_{X,Y}(Y - f(X))^2$$

  and the empirical risk

$$\hat{\mathcal{R}}(f) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$$

  Sometimes we use absolute loss $l(y, \hat{y}) = |y - \hat{y}|$ for robust optimization (since the penalty for large errors is smaller).

1.1.3 Bayes Risk

After the definition of performance criterion for supervised learning, what is the best prediction function f regardless of the data? The answer is, the Bayes risk and Bayes predictor.

Using the the law of iterated expecation, we have

$$\mathcal{R}(f) = \mathbb{E}\big[l(Y, f(X))\big] = \mathbb{E}\Big[\mathbb{E}\big[l(Y, f(X)) \mid X\big]\Big] = \int_{\mathcal{X}} \mathbb{E}\big[l(Y, f(X)) \mid X = x\big] dP_X(x)$$

where

$$\mathcal{R}(f; x) = \mathbb{E}[l(Y, f(X)) \mid X = x]$$

can be viewed as conditional risk, which is a deterministic function.

Proposition 1.1 (Bayes Predictor and Bayes Risk)**.** The expected risk is minimized at a Bayes predictor $f^* : \mathcal{X} \to \mathcal{Y}$ satisfying for all $x \in \mathcal{X}$,

$$f^*(x) \in \operatorname*{arg\,min}_{f(X)\in\mathcal{Y}} \mathbb{E}\big[l(Y, f(X)) \mid X = x\big] \tag{1.3}$$

The Bayes risk $\mathcal{R}^*$ is the risk of all Bayes predictors and is equal to

$$\mathcal{R}^* = \mathbb{E}_X\Big[\inf_{f(X)\in\mathcal{Y}} \mathbb{E}\big[l(Y, f(X)) \mid X\big]\Big] \tag{1.4}$$

Remark 1.1. At every point $x \in \mathcal{X}$ we have a minimizer $z^* \in \mathcal{Y}$. We unite all (x, z^*) pair, we can construct a maps from $\mathcal{X}$ to $\mathcal{Z}^*$, where $\mathcal{Z}$ is the set of all minimizer z^* at each point x. We denotes such map as

$f^* : \mathcal{X} \to \mathcal{Z}^*$. The Bayes risk is then the probability weighted average ($P(x)$) of the conditional loss at each point x.

Proof. By definition, we have

$$\begin{aligned}
\mathcal{R}^* = \mathcal{R}(f^*) &= \mathbb{E}\big[l(Y, f^*(X))\big] \\
&= \mathbb{E}\Big[\mathbb{E}\big[l(Y, f^*(X)) \mid X\big]\Big] \\
&= \mathbb{E}\Big[\inf_{f(X)\in\mathcal{Y}} \mathbb{E}\big[l(Y, f(X)) \mid X\big]\Big]
\end{aligned}$$

□

Note that the Bayes predictor is not always unique, but that all lead to the same Bayes risk (e.g. in binary classification when $\mathbb{P}(Y = 1 \mid X) = 1/2$), and the Bayes risk is usually nonzero, unless the dependence between X and Y is deterministic. Given a supervised learning problem, the Bayes risk is the optimal performance; we define the excess risk as the deviation with respect to the optimal risk.

Proposition 1.2 (Excess Risk)**.** The excess risk of a function $f : \mathcal{X} \to \mathcal{Y}$ is equal to $\mathcal{R}(f) - \mathcal{R}^*$, and it is always non-negative.

Proof. We prove the propsition under the setting of binary classification with loss $l(y, \hat{y}) = \mathbb{1}(y \neq \hat{y})$. For any fixed $X = x, x \in \mathcal{X}$, the conditional risk is

$$\begin{aligned}
\mathcal{R}(f; x) &= \mathbb{E}[\mathbb{1}(Y \neq f(X)) \mid X = x] \\
&= \mathbb{P}(Y \neq f(X) \mid X = x) \\
&= 1 - \mathbb{P}(Y = 1, f(X) = 1 \mid X = x) - \mathbb{P}(Y = -1, f(X) = -1 \mid X = x) \\
&= 1 - \mathbb{P}(Y = 1 \mid X = x)\mathbb{P}(f(X) = 1 \mid X = x) - \mathbb{P}(Y = -1 \mid X = x)\mathbb{P}(f(X) = -1 \mid X = x) \\
&= 1 - \eta(x)\mathbb{E}\big[\mathbb{1}(f(x) = 1)\big] - (1 - \eta(x))\mathbb{E}\big[\mathbb{1}(f(x) = -1)\big]
\end{aligned}$$

Hence, for $X = x, x \in \mathcal{X}$, the difference of excess conditional risk is

$$\begin{aligned}
\mathcal{R}(f; x) - \mathcal{R}(f^*; x) &= \mathbb{E}\big[\mathbb{1}(Y \neq f(X)) \mid X = x\big] - \mathbb{E}\big[\mathbb{1}(Y \neq f^*(X)) \mid X = x\big] \\
&= \mathbb{P}(Y \neq f(X) \mid X = x) - \mathbb{P}(Y \neq f^*(X) \mid X = x) \\
&= \eta(x)\Big(\mathbb{E}\big[\mathbb{1}(f^*(x) = 1)\big] - \mathbb{E}\big[\mathbb{1}(f(x) = 1)\big]\Big) + (1 - \eta(x))\Big(\mathbb{E}\big[\mathbb{1}(f^*(x) = 0)\big] - \mathbb{E}\big[\mathbb{1}(f(x) = 0)\big]\Big) \\
&= (2\eta(x) - 1)\Big(\mathbb{E}\big[\mathbb{1}(f^*(x) = 1)\big] - \mathbb{E}\big[\mathbb{1}(f(x) = 1)\big]\Big) \\
&\geq 0
\end{aligned}$$

The last inequality is due to the fact that

- if $\eta(x) \geq 1/2$, $2\eta(x) - 1 \geq 0$ and $\mathbb{E}[\mathbb{1}(f^*(x) = 1)] = 1 \geq \mathbb{E}[\mathbb{1}(f(x) = 1)]$; the product of two nonnegatives are nonnegative
- if $\eta(x) \leq 1/2$, $2\eta(x) - 1 \leq 0$ and $\mathbb{E}[\mathbb{1}(f^*(x) = 1)] = 0 \leq \mathbb{E}[\mathbb{1}(f(x) = 1)]$; the product of two negatives are nonnegative

Therefore, we have shown that $\mathcal{R}(f) \geq \mathcal{R}(f^*)$ for any function f. □

Therefore, machine learning is ”trivial”: given the distribution $Y \mid X$ for any $X = x$, the optimal predictor is known. The difficulty will be that this distribution is unknown.

- **Binary classification**. the Bayes predictor for $\mathcal{Y} = \{-1, 1\}$ and $l(y, \hat{y}) = \mathbb{1}(y \neq \hat{y})$ is

$$f^* = \operatorname{sgn}(2\eta(x) - 1) = \begin{cases} +1, & \text{if } \eta(x) \geq 1/2 \\ -1, & \text{otherwises} \end{cases} \tag{1.5}$$

  where $\eta(x) = \mathbb{P}(Y = 1 \mid X = x)$. Note that $\eta(x) \geq 1/2$ is equivalent to

$$\frac{\mathbb{P}(Y = +1 \mid X = x)}{\mathbb{P}(Y = -1 \mid X = x)} \geq 1$$

  The corresponding Bayes risk is

$$\mathcal{R}^* = \mathbb{P}(Y \neq f^*(X)) = \mathbb{E}\big[\min\{\eta(x), 1 - \eta(x)\}\big]$$

  Proof. The conditional risk is

$$\begin{aligned} \mathcal{R}(f; x) &= \mathbb{E}\big[\mathbb{1}(Y \neq f(X)) \mid X = x\big] \\ &= \mathbb{P}(Y \neq f(X) \mid X = x) \\ &= \mathbb{P}(Y = 1, f(X) = -1 \mid X = x) + \mathbb{P}(Y = -1, f(X) = 1 \mid X = x) \\ &= \mathbb{P}(Y = 1 \mid X = x)\mathbb{P}(f(x) = -1) + \mathbb{P}(Y = -1 \mid X = x)\mathbb{P}(f(x) = 1) \\ &= \eta(x)\mathbb{P}(f(x) = -1) + (1 - \eta(x))\mathbb{P}(f(x) = 1) \end{aligned}$$

  To minimize $\mathcal{R}(f; x)$, we wish the function $f : \mathcal{X} \to \{-1, 1\}$ satisfying

$$\mathcal{R}(f; x) = \begin{cases} \eta(x) & \text{if } \eta(x) \leq 1/2 \\ 1 - \eta(x) & \text{if } \eta(x) > 1/2 \end{cases}$$

  Therefore, we can simply let

$$f^*(x) = \operatorname*{arg\,min}_{f(x) \in \{-1,1\}} \mathcal{R}(f; x) = \operatorname{sgn}(2\eta(x) - 1) = \begin{cases} -1 & \text{if } \eta(x) \leq 1/2 \\ +1 & \text{if } \eta(x) > 1/2 \end{cases}$$

  as the Bayes predictor. The Bayes risk is therefore

$$\begin{aligned} \mathcal{R}^* &= \mathbb{E}_X\big[\mathcal{R}(f^*; X)\big] \\ &= \mathbb{E}_X\Big[\eta(X)\mathbb{P}\big(\eta(X) \leq 1/2\big) + (1 - \eta(X))\mathbb{P}\big(\eta(X) > 1/2\big)\Big] \\ &= \mathbb{E}_X\Big[\min\{\eta(X), 1 - \eta(X)\}\Big] \end{aligned}$$

  □

- **Regression**. the Bayes predictor for $\mathcal{Y} = \mathbb{R}$ and $l(y, \hat{y}) = (y - \hat{y})^2$ is such that

$$f^*(x) = \mathbb{E}[Y \mid X = x] \tag{1.6}$$

  The corresponding Bayes risk is

$$\mathcal{R}^* = \mathcal{R}(f^*) = \mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X]\big)^2\Big]$$

Proof. The conditional risk of given function $f : \mathcal{X} \to \mathbb{R}$ is

$$\begin{aligned}
\mathcal{R}(f;x) &= \mathbb{E}[(Y - f(X))^2 \mid X = x] \\
&= \mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X = x] + \mathbb{E}[Y \mid X = x] - f(X)\big)^2 \mid X = x\Big] \\
&= \mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X = x]\big)^2 \mid X = x\Big] + \mathbb{E}\Big[\big(f(X) - \mathbb{E}[Y \mid X = x]\big)^2 \mid X = x\Big] \\
&\quad + 2\mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X = x]\big)\big(\mathbb{E}[Y \mid X = x] - f(X)\big) \mid X = x\Big]
\end{aligned}$$

Notice that

$$\begin{aligned}
&\mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X = x]\big)\big(\mathbb{E}[Y \mid X = x] - f(X)\big) \mid X = x\Big] \\
=&\big(\mathbb{E}[Y \mid X = x] - f(x)\big)\mathbb{E}\Big[Y - \mathbb{E}[Y \mid X = x] \mid X = x\Big] \\
=&\big(\mathbb{E}[Y \mid X = x] - f(x)\big)\big(\mathbb{E}[Y \mid X = x] - \mathbb{E}[Y \mid X = x]\big) \\
=&0
\end{aligned}$$

We have

$$\begin{aligned}
f^*(x) &= \arg\min_{f(X) \in \mathbb{R}} \mathbb{E}[(Y - f(X))^2 \mid X = x] \\
&= \arg\min_{f(X) \in \mathbb{R}} \mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X = x]\big)^2 \mid X = x\Big] + \mathbb{E}\Big[\big(f(X) - \mathbb{E}[Y \mid X = x]\big)^2 \mid X = x\Big] \\
&= \mathbb{E}[Y \mid X = x]
\end{aligned}$$

and the Bayes risk is

$$\mathcal{R}^* = \mathbb{E}_X[\mathcal{R}(f^*; X)] = \mathbb{E}\big[(Y - f^*(X))^2\big] = \mathbb{E}\Big[\big(Y - \mathbb{E}[Y \mid X]\big)^2\Big]$$

□

1.2 Learning from Data

The decision theory framework outlined in the previous section gives a test performance criterion and optimal predictors, but it depends on the full knowledge of the *test distribution* $P(x, y)$. We now briefly review how we can obtain good prediction functions from *training data*, that is data sampled i.i.d. from the same distribution $P(x, y)$. There are two main classes prediction algorihms:

- Local Averaging Methods
  - Nearest-neighbors
- Empirical Risk Minimization
  - Linear least-squares regression
  - Kernel methods
  - Sparse methods
  - Neural networks

1.2.1 Local Averaging Methods

Given n observations $(x_1, y_1), \dots, (x_n, y_n)$ where $\mathcal{X}$ is a metric space and $\mathcal{Y} \in \{0, 1\}$, a new point x^{test} is classified by a majority vote among the k-nearest neighbor of x^{test}.

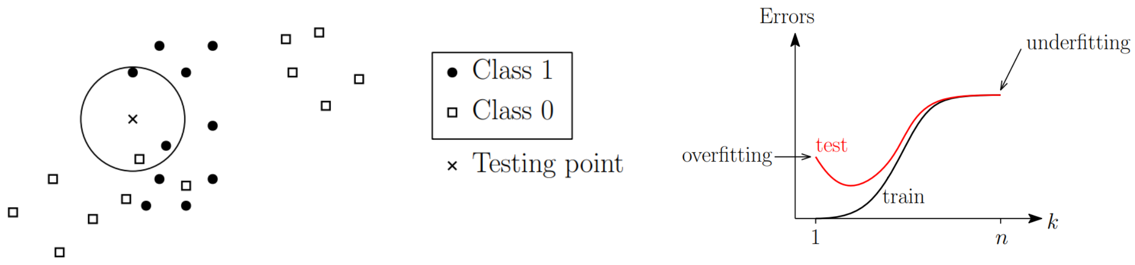


Figure 1: k-nearest-neighbor

- Pros:
  (a) no optimization or training
  (b) often easy to implement
  (c) can get very good performance in low dimensions (in particular for non-linear dependences between x and y)
- Cons:
  (a) slow at query time: must pass through all training data at each testing point (there are ways to reduce complexity)
  (b) bad for high-dimensional data (curse of dimensionality)
  (c) the choice of local *distance function* is crucial
  (d) the choice of ”width” parameter or k has to be performed

1.2.2 Empirical Risk Minimiation

Consider a parameterized family of prediction functions $f_\theta : \mathcal{X} \to \mathcal{Y}$ for $\theta \in \Theta$ and minimize the empirical risk with respect to $\theta \in \Theta$:

$$\hat{\mathcal{R}}(f_\theta) = \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i))$$

this defines the estimator

$$\hat{\theta} \in \arg\min_{\theta \in \Theta} \hat{\mathcal{R}}(f_\theta)$$

and a function $f_{\hat{\theta}} : \mathcal{X} \to \mathcal{Y}$.

- Pros:
  (a) can be relatively easy to optimize (simple derivation and numerical algebra), many algorithms avaliable (mostly based on gradient descent)
  (b) can be applied in any dimension (if a reasonable feature vector is available)

- Cons:
  (a) can be relatively hard to optimize (e.g. neural networks)
  (b) need a good feature vector for linear methods
  (c) dependence on parameters can be complex (e.g. neural networks)
  (d) need some capacity control to avoid overfitting
  (e) how to parameterize functions with values in $\{0,1\}$ (convex surrogates)
- Example: linear least-squares regression

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^\top \phi(x_i))^2$$

here $f_\theta = \theta^\top \phi(x_i)$ is linear in some feature vector $\phi(x) \in \mathbb{R}^d$ (no need for $\mathcal{X}$ to be a vector space). The vector $\phi(x)$ can be quite large.

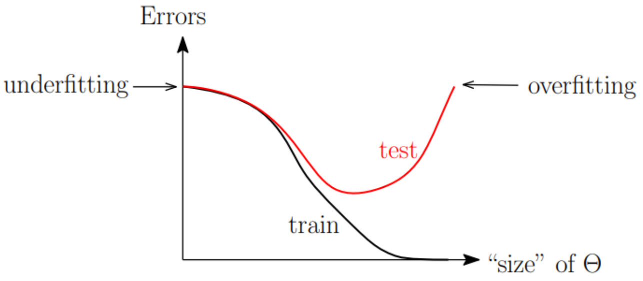


Figure 2: empirical risk

- **Risk decompmosition**

  Given any $\hat{\theta} \in \Theta$, we can weite the excess risk of $f_{\hat{\theta}}$ as:

$$\begin{aligned}\mathcal{R}(f_{\hat{\theta}}) - \mathcal{R}^* &= \left\{\mathcal{R}(f_{\hat{\theta}}) - \inf_{\theta\in\Theta}\mathcal{R}(f_\theta)\right\} + \left\{\inf_{\theta\in\Theta}\mathcal{R}(f_\theta) - \mathcal{R}^*\right\} \\ &= \text{estimation error} \quad + \quad \text{approximation error}\end{aligned}$$

  - The *estimation error* is typically random, becasue the function $f_{\hat{\theta}}$ is random (depend on random training data). It is typically decreasing in n (more data, less uncertainty), and usually goes up when Θ grows.
  - The *approximation error* does not depend on the chosen of $f_{\hat{\theta}}$, and is also independent of traning size n. It depends only on the class of functions parameterized by $\theta \in \Theta$, and hence it is always a determinsitic function. When Θ grows, the approximation error goes down, and to zero if arbitrary functions can be approximated arbitrary well by the function f_θ.

  Typically, for any $\hat{\theta} \in \Theta$, the *estimation error* is often decomposed as

$$\begin{aligned}\left\{\mathcal{R}(f_{\hat{\theta}}) - \mathcal{R}(f_{\theta^*})\right\} &= \left\{\mathcal{R}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\hat{\theta}})\right\} + \left\{\hat{\mathcal{R}}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\theta^*})\right\} + \left\{\hat{\mathcal{R}}(f_{\theta^*}) - \mathcal{R}(f_{\theta^*})\right\} \\ &\leq 2\sup_{\theta\in\Theta}\left|\hat{\mathcal{R}}(f_\theta) - \mathcal{R}(f_\theta)\right| \quad + \quad \text{empirical optimizati error}\end{aligned}$$

where θ^* is a minimizer on Θ. The uniform deviation grows with the "size" of Θ, and usually decays with n.

- **Capacity control**

  In order to avoid overfitting, we need to make sure that the set of allowed functions is not too large, by typically reducing the number of parameters, or by restricting the norm of predictors (thus by reducing the "size" of Θ): this typically leads to constrained optimization, and allows for risk decompositions as done above.

  This can be done by regularization, that is, minimizing the follow:

  $$\hat{\mathcal{R}}(f_\theta) + \lambda\Omega(\theta) = \frac{1}{n}\sum_{i=1}^{n} l(y_i, f_\theta(x_i)) + \lambda\Omega(\theta)$$

  where $\Omega(\theta)$ controls the complexity of f_θ. The main example is ridge regression:

  $$\min_{\theta\in\mathbb{R}^d} \quad \frac{1}{n}\sum_{i=1}^{n}\big(y_i - \theta^\top\phi(x_i)\big)^2 + \lambda||\theta||_2^2$$

  this is often easier to optimization, but harder to analyze.

  Note: There is a difference between parameters (e.g., θ) learned on the training data and hyperparameters (e.g., λ) learned on the validation data

1.3 Statistical Learning Theory

The goal of learning theory is to provide some guarantess of performance on unseen data. A common assumption is that the samples $S_n(P) = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ are obtained as i.i.d. observations from some unknown distribution P from a family $\mathcal{P}$.

An algorithm $\mathcal{A}$ is a mapping from $S_n(P)$ (could be any size n) to a function from $f : \mathcal{X} \mapsto \mathcal{Y}$. The risk depends on the probability $P \in \mathcal{P}$, as $\mathcal{R}_P(f)$. The goal is to find $\mathcal{A}$ such that the risk

$$\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big) - \mathcal{R}_P^*$$

is small enough, where $\mathcal{R}_P^*$ is the Bayes risk with respect to joint distribution $P(X, Y)$. Here we assume that $S_n(P)$ is sampled from P, where $P \in \mathcal{P}$ is unknown. Moreover, the risk is random because S_n is random.

1.3.1 Measures of Performance

There are several ways of dealing with the randomness of the risk in order to obtain a criterion.

- **Expected Error**: we measure the performance of algorithm as

  $$\mathbb{E}\Big[\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big)\Big]$$

  where the expectation is with respect to the training data. An algorithm $\mathcal{A}$ is called *consistent in expectation* for the distribution P, if

  $$\mathbb{E}\Big[\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big)\Big] - \mathcal{R}_P^* \to 0$$

  when n tends to infinity.

- **Probably Approximately Correct (PAC) Learning**: for a given $\delta \in (0,1)$ and $\varepsilon > 0$

  $$\mathbb{P}\Big(\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big) - \mathcal{R}_P^* \leq \varepsilon\Big) \geq 1 - \delta$$

  The crux is to find ε which is as small as possible (typically as a function of δ). An algorithm $\mathcal{A}$ is called consistent in PAC for the distribution P, if for any $\varepsilon > 0$, there exists $\delta_n \in (0,1)$, such that

  $$\mathbb{P}\Big(\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big) - \mathcal{R}_P^* \leq \varepsilon\Big) \geq 1 - \delta_n$$

  and the sequence δ_n goes to zero as $n \to \infty$.

1.3.2 Some Notions in Learning Problems

Definition 1.3 (Uniform Consistency)**.** An algorithm is called universally consistent (in expectation) if for all distributions P on (X, Y), the algorithm $\mathcal{A}$ is consistent in expectation with respect to distribution P.

Most often, we want to study uniform consistency within a class $\mathcal{P}$ of distributions satisfying some regularities. We thus aim at finding an algorithm $\mathcal{A}$ such that

$$\sup_{P \in \mathcal{P}} \; \mathbb{E}\Big\{\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big) - \mathcal{R}_P^*\Big\}$$

is as small as possible. We will see the details in Section 3 and 4.

Definition 1.4 (Minimax Risk)**.** The minimax risk is defined as

$$\inf_{\mathcal{A}} \sup_{P \in \mathcal{P}} \; \mathbb{E}\Big\{\mathcal{R}_P\big(\mathcal{A}(S_n(P))\big) - \mathcal{R}_P^*\Big\} \tag{1.7}$$

The minimax risk is typically a function of the sample size n, the properties of $\mathcal{X}, \mathcal{Y}$ and the distribution space $\mathcal{P}$. In order to compute the estimates of minimax risk, several techniques exist:

- Upper-bounding: one given algorithm with a convergence proof provides an upper-bound on the optimal performance
- Lower-bounding: in some setups, it is possible to show that the infimum over all algorithms is greater than a certian quantity.

The ML researcher are happy when upper-bounds and lower-bounds match (up to constant factors).

- **Non-asymptotic Analysis**

  The analysis can be "non-asymptotic", with an upper-bound with explicit dependence on all quantities; the bound is then valid for all n, even if sometimes vacuous.

- **Asymptotic Analysis**

  The analysis can also be "asymptotic", where for examples n goes to infinity and limits are taken (alternatively, several quantities can be made to grow simultaneously).

What (arguably) matters most here is the dependence of these **rates** on the problem, not the choice of "in expectation" vs. in "high probability", or "asymptotic" vs. "non-asymptotic", as long as the problem parameters explicitly appear.

1.3.3 No Free Lunch Theorems

Although it may be tempting to define the optimal learning algorithm that works optimally for all distributions, this is impossible. **In other words, learning is not possible without assumptions**.

The following theorems shows that for any algorithm, for a fixed n, there is a data distribution P that makes the algorithm useless

Theorem 1.1 (No Free Lunch - Fixed n)**.** Consider the binary classification with 0-1 loss, with $\mathcal{X}$ infinite. Let $\mathcal{P}$ denote the set of all probability distributions on $\mathcal{X} \times \{0, 1\}$. For any $n > 0$ and learning algorithm $\mathcal{A}$,

$$\sup_{P \in \mathcal{P}} \left\{ \mathbb{E}_{S_n} \left[\mathcal{R}_P \big(\mathcal{A}(S_n(P)) \big) \right] - \mathcal{R}_P^* \right\} \geq 1/2$$

The proof see Bach 2021. The folliwng theroem is much stronger, as it more convincingly shows that learning can be arbitrarily slow without assumption.

Theorem 1.2 (No Free Lunch - Sequence of Errors)**.** Consider the binary classification with 0-1 loss, with $\mathcal{X}$ infinite. Let $\mathcal{P}$ denote the set of all probability distributions on $\mathcal{X} \times \{0, 1\}$. For any decreasing sequence a_n tending to zero and such that $a_1 \leq 1/16$, for any learning algorithm $\mathcal{A}$, there exists $P \in \mathcal{P}$, such that for all $n \geq 1$,

$$\mathbb{E}_{S_n} \left[\mathcal{R}_P \big(\mathcal{A}(S_n(P)) \big) \right] - \mathcal{R}_P^* \geq a_n$$

2 Convexification of the Risk

Before looking at the necessary probabilistic tools, we will first show how problems where the output space is not a vector space, such as binary classification with $y = \{-1, 1\}$, can be reformulated with so-called convex surrogates of loss functions.

Remark 2.1 (Motivation of Risk Convexificatoin)**.** As our goal is to estimate a binary-valued function, the first idea that comes into mind is to minimize the empirical risk over a hypothesis space of binary-valued functions. However, this approach leads to a combinatorial problem which can be computationally intractable and moreover, it is not clear how to control the capacity for these type of hypothesis spaces. Learning a real-valued function instead through the problem the framework of convex surrogates simplifies and overcomes this problem as it convexifies the problem and classical penalty-based regularization techniques can be used for theoretical analysis and for algorithms.

Instead of learning $f : \mathcal{X} \mapsto \{-1, 1\}$, we will thus learn a function $g : \mathcal{X} \mapsto \mathbb{R}$ and define $f(x) = \operatorname{sgn}(g(x))$ where

$$\operatorname{sgn}(a) = \begin{cases} +1 & \text{if} \quad a \geq 0 \\ -1 & \text{if} \quad a < 0 \end{cases}$$

The risk of the function $f = \operatorname{sgn} \circ g$, still denoted $\mathcal{R}(g)$, is then equal to

$$\mathcal{R}(g) = \mathbb{P}\big(\operatorname{sgn}(g(x) \neq y)\big) = \mathbb{E}\big[\mathbb{1}(g(x) \neq y)\big] = \mathbb{E}\big[\mathbb{1}(yg(x) < 0)\big] = \mathbb{E}\big[\phi_{0-1}(yg(x))\big]$$

where $\phi_{0-1} : \mathbb{R} \mapsto \mathbb{R}$, with $\phi_{0-1}(u) = \mathbb{1}(u < 0)$ is called the "margin-based" $0-1$ loss function. For empirical risk minimization, we then miniize the empirical risk

$$\hat{\mathcal{R}}(g) = \frac{1}{n} \sum_{i=1}^{n} \phi_{0-1}(y_i g(x_i))$$

with respect to $g : \mathcal{X} \mapsto \mathbb{R}$. However, the function ϕ_{0-1} is not continuous (and thus also non-convex) and leads to difficult optimization problems.

2.1 Convex Surrogates

A key concept in machine learning is the use of convex surrogates, where we replace ϕ_{0-1} by another function ϕ with better numerical properties (all will be convex). Instead of minimizing the classical risk $\mathcal{R}(g)$ or its empirical version $\hat{\mathcal{R}}(g)$, one then minimizes the ϕ-risk (and its empirical version) defiend as

$$\mathcal{R}_\phi(g) = \mathbb{E}\big[\phi(yg(x))\big]$$

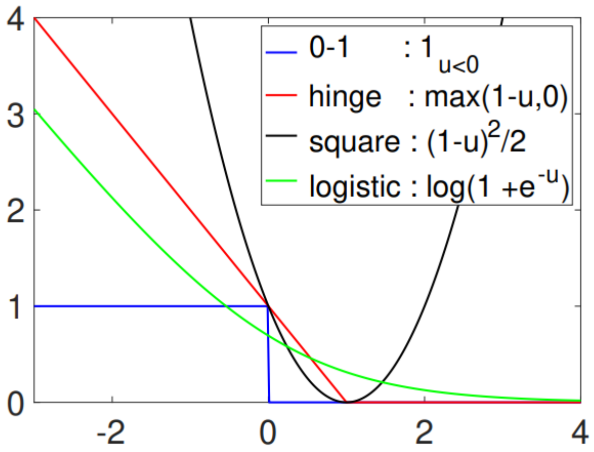
and

$$\hat{\mathcal{R}}_\phi(g) = \frac{1}{n} \sum_{i=1}^{n} \phi(yg(x))$$

- **Quadratic loss**. $\phi(u) = (u-1)^2$ leading to

  $$\begin{aligned} \phi(yg(x)) &= (yg(x) - 1)^2 = (yg(x) - y^2)^2 = y^2(g(x) - y)^2 \\ &= (y - g(x))^2 = (g(x) - y)^2 \end{aligned}$$

  with the notice that $y^2 = 1$. Hence, we get leas-squares.



- **Logistic loss**. $\phi(u) = \log(1 + e^{-u})$, leading to

$$\phi(yg(x)) = \log(1 + e^{-yg(x)}) = -\log\left(\frac{1}{1 + e^{-yg(x)}}\right) = -\log\sigma(yg(x))$$

  where $\sigma(\nu) = 1/(1 + e^{-\nu})$ is the sigmoid function. Note the link with maximum likelihood estimation, where we define the model through

$$\mathbb{P}(y = 1 \mid x) = \sigma(f(x)) \quad \text{and} \quad \mathbb{P}(y = -1 \mid x) = \sigma(-f(x)) = 1 - \sigma(f(x))$$

- **Hinge loss**. $\phi(u) = \max(1 - u, 0)$, with linaer predictors, this leads to the support vector machine, and $yf(x)$ is often called the "margin" in this context. This loss has a geometric interpretation.

- **Squared Hinge loss**. $\phi(u) = \max(1 - u, 0)^2$, this is a smooth counterpart to the regular hinge loss.

2.2 Geometric Interpretation of the Support Vector Machine

We consider n observations $(x_i, y_i) \in \mathbb{R}^d \times \{-1, 1\}$ for $i = 1, \ldots, n$.

Separable data. We first assume that the data are separable by an affine hyperpalne, that is, there exist $\omega \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that for all $i \in \{1, \ldots, n\}$,

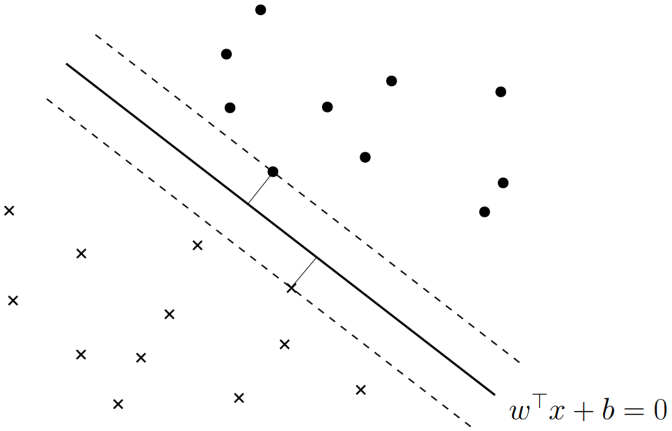
$$y_i(\omega^\top x_i + b) > 0$$

Among the infinitely many separating hyperplane, we aim at selecting the one for which closet point from the dataset is farthest.

The distance from x_i to the hyperplane $\{x \in \mathbb{R}^d, \omega^\top x + b = 0\}$ is equal to $\frac{|\omega^\top x_i + b|}{||\omega||_2}$, and thus, this minimal distance is

$$\underset{x_i}{\text{minimize}} \quad \frac{y_i(\omega^\top x_i + b)}{||\omega||_2}$$

and we thus aim at maximizing this quantity over ω and b. Because of the invariance by rescaling ω and b,



that is, we can rescale (ω, b) pair such that

$$\underset{x_i}{\text{minimize}} \quad \frac{y_i(\omega^\top x_i + b)}{||\omega||_2} = \frac{1}{||\omega||_2}$$

Then this problem is equivalent to

$$\begin{aligned} \underset{\omega \in \mathbb{R}^d,\ b \in \mathbb{R}}{\text{minimize}} \quad & \frac{1}{2}||\omega||_2^2 \\ \text{subject to} \quad & y_i(\omega^\top x_i + b) \geq 1, \quad \forall\ i \in \{1, \dots, n\} \end{aligned} \tag{2.1}$$

General data. When data may not separated by an hyperplane, then we can introduce so-called ”slack variables” $\xi_i \geq 0, i = 1, \dots, n$, allowing the constraint $y_i(\omega^\top x_i + b) \geq 1$ to be not satisfied, by introducing instead the constraint

$$y_i(\omega^\top x_i + b) \geq 1 - \xi_i$$

The overall amount of slack is then minimized, leading tot he following problem (with $C > 0$)

$$\begin{aligned} \underset{\omega \in \mathbb{R}^d, b \in \mathbb{R}, \xi \in \mathbb{R}^n}{\text{minimize}} \quad & \frac{1}{2}||\omega||_2^2 + C \sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & y_i(\omega^\top x_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \quad \forall\ i \in \{1, \dots, n\} \end{aligned} \tag{2.2}$$

With $\lambda = \frac{1}{nC}$, the problem above is equivalent to

$$\underset{\omega \in \mathbb{R}^d, b \in \mathbb{R}}{\text{minimize}} \quad \frac{1}{n} \sum_{i=1}^{n} \left(1 - y_i(\omega^\top x_i + b)\right)^+ + \frac{\lambda}{2}||\omega||_2^2$$

which is exactly an l_2-regularized empirical risk minimization with the hinge loss, for the prediction function $f(x) = \omega^\top x + b$.

Lagrange dual. The problem in Eq.2.2 is a linearly constrained convex optimmization problem, and can be analyzed using Lagrangian duality. We consdier non-negative Lagrange multipliers α_i and β_i, $i \in \{1, \dots, n\}$ and the following Lagrangian

$$\mathcal{L}(\omega, b, \xi, \alpha, \beta) = \frac{1}{2}||\omega||_2^2 + C\sum_{i=1}^{n} \xi_i - \sum_{i=1}^{n} \alpha_i \big(y_i(\omega^\top x_i + b) - 1 + \xi_i\big) - \sum_{i=1}^{n} \beta_i \xi_i$$

Minimizing with respect to $\xi \in \mathbb{R}^n$ leads to the constraints

$$\alpha_i + \beta_i = C \quad \forall\ i \in \{1, \dots, n\}$$

while minimizing with respect to b leads to the constraints

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

and finally minimizing with respect to ω tells us

$$\omega = \sum_{i=1}^{n} \alpha_i y_i x_i$$

Substitute these constraints back to Lagrangian we get the dual function and dual optimizaton problem

$$\begin{aligned} \underset{\alpha \in \mathbb{R}^n}{\text{maximize}} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^\top x_j \\ \text{subject to} \quad & \sum_{i=1}^{n} \alpha_i y_i = 0 \\ & \alpha_i \in [0, C] \quad \forall\ i \in \{1, \dots, n\} \end{aligned} \tag{2.3}$$

As we will show in the future that all l_2-regularized learning problems with linear predictors, the optimization problem only depends on the dot-products

$$x_i^\top x_j \quad \forall\ i, j = 1, \dots, n$$

and the optimal predictor can be wriiten as a linear combination of input data points $x_i, i = 1, \dots, n$.

Support vector. For optimal primal and dual variables, the "complementary slackness" conditions for linear inequality constraints lead to

$$\alpha_i \big(y_i(\omega^\top x_i + b) - 1 + \xi_i\big) = 0$$

and

$$\beta_i \xi_i = (C - \alpha_i)\xi_i = 0$$

This implies that $\alpha_i = 0$ as soon as $y_i(\omega^\top x_i + b) < 1$, and thus many of the α_i are equal to zero, and the optimal predictor is a linear combination of only a few of the data point x_i's which are then called "support vectors".

2.3 Conditional Surrogate Risk and Classification Calibration

Most of the convex surrogates Φ are upper-bounds on the $0-1$ loss, and all can be made so with rescaling. Using this as the sole justification of the good performance of a convex surrogate is misleading justification, with the exception of problems with almost surely zero loss for the Bayes predictor (which is only possible when the Bayes risk is zero).

If we denote $\eta(X) = \mathbb{P}(Y = 1 \mid X) \in [0, 1]$, then we have, $\mathbb{E}[Y \mid X] = 2\eta(x) - 1$ and as in Section 1.1,

$$\mathcal{R}(g) = \mathbb{E}\Big[\Phi_{0-1}(Yg(X))\Big] = \mathbb{E}\Big[\mathbb{E}\big[\mathbb{1}(Y \neq g(X)) \mid X\big]\Big] \geq \mathbb{E}\Big[\min\big\{\eta(X), 1 - \eta(X)\big\}\Big] = \mathcal{R}^*$$

and one of the best classifier is

$$f^*(X) = \operatorname{sgn}(2\eta(X) - 1)$$

Note that there are many potential other functions $g(x)$ than $2\eta(X) - 1$ so that $f^*(X) = \operatorname{sgn}(g(X))$ is optimal. The first (minor) reason is the arbitrary choice of prediction for the tie $\eta(X) = 1/2$. The other reason is that $g(X)$ simply has to have the same sign as $2\eta(X) - 1$, which leads to many possibilities beyond $2\eta(X) - 1$.

In order to study the impact of using the Φ-risk, we first look at the conditional risk for a given X (as for the 0-1 loss, the function that g that will minimize the Φ-risk can be determined by looking at each x separately).

Definition 2.1 (Conditional Φ-risk)**.** Let $g : \mathcal{X} \to \mathbb{R}$, we define the conditional Φ-risk as

$$\mathbb{E}\big[\Phi(Yg(X)) \mid X\big] = \eta(X)\Phi(g(X)) + \big(1 - \eta(X)\big)\Phi(-g(X)) := C_{\eta(X)}\big(g(X)\big) \tag{2.4}$$

with

$$C_\eta(\alpha) = \eta\Phi(\alpha) + (1 - \eta)\Phi(-\alpha)$$

The least we can expect from a convex surrogate is that in the population case, where all X's decouple, the optimal $g(X)$ obtained by minimizing the conditional Φ-risk exactly leads to the same prediction as the Bayes predictor (at least when this prediction is unique). In other words, since the prediction is $\operatorname{sgn}(g(X))$, we want that for any $\eta \in [0, 1]$:

$$\begin{aligned} &\text{(positive optimal prediction)}, \quad \eta > 1/2 \quad \Leftrightarrow \quad \operatorname*{arg\,min}_{\alpha\in\mathbb{R}} \ C_\eta(\alpha) \subset \mathbb{R}_+ \\ &\text{(negative optimal prediction)}, \quad \eta < 1/2 \quad \Leftrightarrow \quad \operatorname*{arg\,min}_{\alpha\in\mathbb{R}} \ C_\eta(\alpha) \subset \mathbb{R}_- \end{aligned} \tag{2.5}$$

A function Φ that satisfies these two statement is said *classification-calibrated*, or simply *calibrated.* It turns out that when Φ is convex, a simple sufficient and necessary condition is avaiable:

Proposition 2.1 (Bartlett, Jordan, and McAuliffe 2006)**.** Let $\Phi : \mathbb{R} \to \mathbb{R}$ convex. Φ calibrated $\Leftrightarrow$ Φ is differentiable at 0 and $\Phi'(0) < 0$.

Proof. Since Φ is convex, so is C_η for any $\eta \in [0, 1]$, and thus we simply consider left and right derivatives at zero too obatin conditions acbout location of minimizers, with the two possibilities below (minimizer in $\mathbb{R}_+$ if and only if the right derivative at zero strictly negative, and minimizre in $\mathbb{R}_-$ if and only if the left

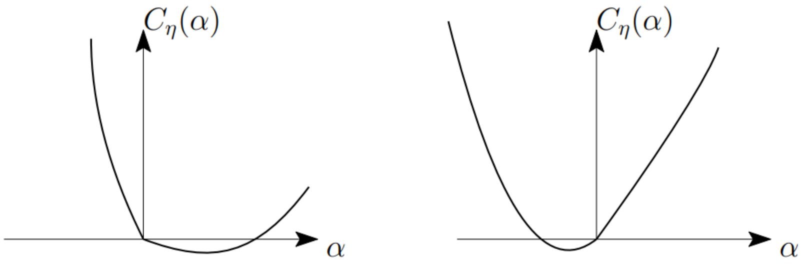


Figure 3: Classification calibration

derivative at zero is strictly positive):

$$\begin{aligned}
\arg\min_{\alpha\in\mathbb{R}} \ C_\eta(\alpha) \subset \mathbb{R}_+ \quad &\Leftrightarrow \quad (C_\eta)_+(0)' = \eta\Phi'_+(0) - (1-\eta)\Phi'_-(0) < 0 \\
\arg\min_{\alpha\in\mathbb{R}} \ C_\eta(\alpha) \subset \mathbb{R}_- \quad &\Leftrightarrow \quad (C_\eta)_-(0)' = \eta\Phi'_-(0) - (1-\eta)\Phi'_+(0) < 0
\end{aligned} \tag{2.6}$$

(a) Assume Φ is calibrated.

By letting η tend to $(1/2)+$ in Eq.(2.6), we have

$$(C_{1/2})_+(0)' = \frac{1}{2}[\Phi'_+(0) - \Phi'_-(0)] \leq 0$$

Since Φ is convex, we always have $\Phi'_+(0) - \Phi'_-(0) \geq 0$. Thus the left and right derivatives are equal, which implies that Φ is differentiable at 0. Then $C'_\eta(0) = (2\eta-1)\Phi'(0)$ and from the first rows of Eq.(2.5) and Eq.(2.6), we need to have $\Phi'(0) < 0$.

(b) Assume Φ is differentiable at 0 and $\Phi'(0) < 0$, then $C'_\eta(0) = (2\eta-1)\Phi'(0)$; Eq.(2.5) are then direct consequnces of Eq.(2.6) by noticing the Fig. 3.

□

Note that the proposition above excludes the convex surrogate $u \mapsto (-u)^+ = \max\{-u, 0\}$, which is not differentiable at zero. From now on, we assume that Φ is calibrated and convex, that is, Φ convex, Φ differentiable in 0, and $\Phi(0) < 0$. We should also notice that if $\Phi(\alpha)$ is symmetric with respect to origin point 0, we have

$$C_{\eta(X)} = (2\eta-1)\Phi(g(X)) \tag{2.7}$$

2.4 Relationship between Risk and Surrogate Risk

Now that we know that for any $x \in \mathcal{X}$, minimizing $C_{\eta(X)}(g(X))$ with respect to $g(X)$ leads to the optimal prediction through $\text{sgn}(g(X))$, we would like to make sure that an explicit control of the excess Φ-risk leads to an explicit control of the original excess risk. In otherwords, we are looking for a monotonic function $H : \mathbb{R}_+ \to \mathbb{R}_+$ such that

$$\mathcal{R}(g) - \mathcal{R}^* \leq H[\mathcal{R}_\Phi(g) - \mathcal{R}^*_\Phi]$$

where $\mathcal{R}^*_\Phi$ is the minimum possible Φ-risk. The function H is often called the **calibration function**.

We first start with a simple lemma expressing the excess risk, as well as an upper bound, that we need for comparison inequalities below.

Lemma 2.1. For any function $g : \mathcal{X} \to \mathbb{R}$, and for a Bayes predictor g^*:

$$\mathcal{R}(g) - \mathcal{R}^* = \mathbb{E}[|2\eta(X) - 1| \cdot \mathbb{1}_{g(X)\cdot g^*(X)<0}]$$

Moreover, we have $\mathcal{R}(g) - \mathcal{R}(g^*) \leq \mathbb{E}|2\eta(X) - 1 - g(X)|$, and as a matter of fact, for any function $b : \mathbb{R} \to \mathbb{R}$ that preserves the sign (that is $b(\mathbb{R}_+) \subset \mathbb{R}_+$ and $b(\mathbb{R}_-) \subset \mathbb{R}_-$), we have

$$\mathcal{R}(g) - \mathcal{R}(g^*) \leq \mathbb{E}[|2\eta(X) - 1 - b(g(X))]$$

Proof. Recall that $\eta(X) = \mathbb{P}(Y = 1 \mid X)$. We express the excess risk as:

$$\begin{aligned}\mathcal{R}(g) - \mathcal{R}(g^*) &= \mathbb{E}\Big[\mathbb{E}\big[\mathbb{1}_{\mathrm{sgn}(g(X))\neq Y} - \mathbb{1}_{\mathrm{sgn}(g^*(X))\neq Y} \mid X\big]\Big] \\ &= \mathbb{E}\Big[\mathbb{E}\big[\mathbb{1}_{\mathrm{sgn}(g(X))\neq 1} - \mathbb{1}_{\mathrm{sgn}(g^*(X))\neq 1} \mid X, Y = 1\big]\eta(X) + \big[\mathbb{1}_{\mathrm{sgn}(g(X))\neq 0} - \mathbb{1}_{\mathrm{sgn}(g^*(X))\neq 0} \mid X, Y = 0\big](1 - \eta(X))\Big]\end{aligned}$$

by definition of the $0 - 1$ loss. For any given $X \in \mathcal{X}$, we can look at the two possible case for the signs of $\eta(X) - 1/2$ and $g(X)$ that lead to different predictions for g and g^*, namely

(a) for $\eta(X) > 1/2$ and $g(X) < 0$, the expectation is $\eta(X) - (1 - \eta(X)) = 2\eta(X) - 1 > 0$; and

(b) for $\eta(X) < 1/2$ and $g(X) > 0$, we get $1 - 2\eta(X) > 0$

By combining these two cases into the condition $g(X) \cdot g^*(X) < 0$ and the condition expectation $|2\eta X - 1|$, we get

$$\mathcal{R}(g) - \mathcal{R}(g^*) = \mathbb{E}\Big[|2\eta(X) - 1| \cdot \mathbb{1}_{\mathrm{sgn}(g(X))\cdot \mathrm{sgn}(g^*(X))<0}\Big]$$

which is just the first result.

For the seoncd result, we simply use the fact that if $g(X) \cdot g^*(X) < 0$, then, by splitting the cases in two (the first one being $\eta(X) > 1/2$ and $g(X) < 0$, the second one being $\eta(X) < 1/2$ and $g(X) > 0$), we get

$$|2\eta(X) - 1| \leq |2\eta(X) - 1 - g(X)|$$

As long as the funcition b presever the sign of $g(X)$, we obtain the last result. □

We see that the excess risk is the expectation of a quantity $|2\eta(X) - 1| \cdot \mathbb{1}_{g(X)\cdot g^*(X)<0}$, which is equal to 0 if the classification is the same as the Bayes predictor and equal to $|2\eta(X) - 1|$ otherwise. On the other hand, the excess conditional Φ-risk is the quantity

$$\eta(X)\Phi(g(X)) + (1 - \eta(X))\Phi(-g(X)) - \inf_{\alpha}\{\eta(X)\Phi(\alpha) + (1 - \eta(X))\Phi(-\alpha)\}$$

which, as a function of $g(X)$, is the deviation between a convex function of $g(X)$ and its minimum value. We simply need to relate it to the quantity $|2\eta(X) - 1| \cdot \mathbb{1}_{g(X)\cdot g^*(X)<0}$ above for any $x \in \mathcal{X}$ and take expectations.

Bartlett, Jordan, and McAuliffe 2006 proposes a general framework. Here we will only consider the hinge loss and smooth losses for simplicity.

- **Hinge Loss**. For the hinge loss $\Phi(\alpha) = (1-\alpha)^+ = \max\{1-\alpha, 0\}$, we can easily compute the minimizer of the conditional Φ-risk (which leads to the minimizer of the Φ-risk). Indeed, we need to minimizer $\eta(X)(1-\alpha)^+ + (1-\eta(X))(1+\alpha)^+$, which is a piecewise affine function with kinks at -1 and 1, with a minimizer attained at $u = 1$ for $\eta(X) > 1/2$, and symmetrically at $u = -1$ for $\eta(X) < 1/2$, with a minimum conditional Φ-risk equal to $2\min\{1-\eta(X), \eta(X)\}$.

  The two excess risks are plotted below for the hinge loss and the 0-1 loss, for $\eta(X) > 1/2$, showing pictorially that the conditional excess Φ-risk is greater than the excess risk.

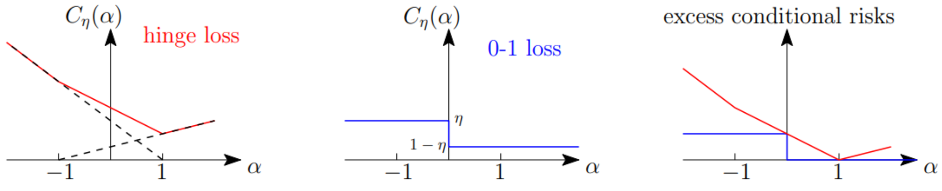
  

  Figure 4: The excess risk of hinge loss and 0-1 loss

  This leads to the calibration function $H(\sigma) = \sigma$ for the hinge loss.

  Note that when the Bayes risk is zero, that is, $\eta(X) \in \{0, 1\}$ almost surely, then using the fact that the hinge loss is an upper-bound on the 0-1 loss is enough to show that the excess risk is less than the excess Φ-risk (indeed, the two optimal risk $\mathcal{R}^*$ and $\mathcal{R}^*_\Phi$ are equal to zero).

- **Smooth Loss**. We consider smooth losses of the form (up to additive and multiplicative constants) $\Phi(v) - a(v) - v$, where $a(v) = \frac{1}{2}v^2$ for the quadratic loss, $a(v) = 2\log(e^{v/2} + e^{-v/2})$ for the logistic loss. We assume that a is even ($a(-v) = a(v)$), $a(0) = 0$, a is β-smooth (that is, $a''(v) \leq \beta$ for all $v \in \mathbb{R}$). This implies that for all $v \in \mathbb{R}$,

  $$a(v) - \alpha v - \inf_{w \in \mathbb{R}} \{a(w) - \alpha w\} \geq \frac{1}{2\beta}|\alpha - a'(v)|^2$$

  leading to

  $$\begin{aligned}\mathcal{R}_\Phi(g) - \mathcal{R}^*_\Phi &= \mathbb{E}[a(g(X)) - (2\eta(X) - 1)g(X) - \inf_{w \in \mathbb{R}} a(w) - (2\eta(X) - 1)w] \\ &\geq \frac{1}{2\beta}\mathbb{E}|2\eta(X) - 1 - a'(g(X))|^2 \quad \text{by property above} \\ &\geq \frac{1}{2\beta}(\mathbb{E}|2\eta(X - 1 - a'(g(X))|)^2 \quad \text{by Jensens's inequality} \\ &\geq \frac{1}{2\beta} \quad \text{by Lemma 2.1}\end{aligned}$$

  This leads to the calibration function $H(\sigma) = \sqrt{\sigma}$ for the square loss and $H(\sigma) = \sqrt{2\sigma}$ for the logistic loss.

Remark 2.2. Show that the function a^* satisfies $a^*\big(\mathcal{R}(g) - \mathcal{R}^*\big) \leq \mathcal{R}_\Phi(g) - \mathcal{R}^*_\Phi$ for any function $g : \mathcal{X} \to \mathbb{R}$.

We can make the following observations:

- For the (non-smooth) hinge loss, the calibration function is identity, so if the excess Φ-risk goes to zero at a certain rate, the excess risk is goes to zero at the same rate; whereas for smooth losses, the upper-bound only ensures a (worse) rate with a square root. Therefore, when going from the excess Φ-risk to the excess risk, that is, after thresholding the function g at zero, the observed rates may be worse.

- Note that the noiseless case when $\eta(X) \in \{0, 1\}$ (zero Bayes risk) leads to stronger calibration function, as well as a series of intermediate ”low-noise” conditions.

2.5 Impact on Approximation Errors

For the same classification problem, several convex surrogates can be used. While the Bayes classifier is always the same, that is,

$$f^*(X) = \mathrm{sgn}(2\eta(X) - 1)$$

the minimmizer of the testing Φ-risk will be different. For example, for the hinge loss, the minimizer $g(X)$ is exactly $\mathrm{sgn}(2\eta(X) - 1)$, while for losses of the form like above $\Phi(v) = a(v) - v$, we have $a'(g(X)) = 2\eta(X) - 1$, and thus for the square loss $g(X) = 2\eta(X) - 1$, while for the logistic loss, one can check that $g(X) = \mathrm{atanh}(2\eta(X) - 1)$ (hyperbolic arc tangent). See example below, with $\mathcal{X} = \mathbb{R}$ and Gaussian class conditional densities.

3 Empirical Risk Minimization

Main Concern. Given a joint distribution $P(X,Y)$ (which is unknown), and n independent and identically distributed observations from $P(X,Y)$, our goal is to learn a function $f:\mathcal{X}\to\mathcal{Y}$ with minimum risk:

$$\mathcal{R}_P(f)=\mathbb{E}_P[l(Y,f(X))]$$

or equivalently minimum excss risk:

$$\mathcal{R}_P(f)-\mathcal{R}_P^*=\mathcal{R}_P(f)-\inf_g \mathcal{R}_P(g)$$

where g is a measurable function. In this section, we introduce the way called empirical risk minimization, and for simplicity we will omit the subscript P in the expected risk $\mathcal{R}$.

3.1 Risk Minimization Decomposition

We consider a family $\mathcal{F}$ of prediction functions $f:\mathcal{X}\to\mathcal{Y}$. Empirical risk mnimization aims at finding

$$\hat{f}\in\arg\min_{f\in\mathcal{F}}\ \hat{\mathcal{R}}(f)=\frac{1}{n}\sum_{i=1}^{n} l(Y_i,f(X_i))$$

where the empirical minimize $\hat{f}$ depends on training sample $S_n=\{(X_1,Y_1),\dots,(X_n,Y_n)\}$ and thus is random. In fact, We can decompose the risk with respect to f as follows into two terms:

$$\begin{aligned}\mathcal{R}(\hat{f})-\mathcal{R}^* &= \Big\{\mathcal{R}(\hat{f})-\inf_{f'\in\mathcal{F}}\mathcal{R}(f')\Big\}+\Big\{\inf_{f'\in\mathcal{F}}\mathcal{R}(f')-\mathcal{R}^*\Big\} \\ &= \text{estimation error} \quad + \quad \text{approximation error}\end{aligned} \tag{3.1}$$

A classical example is the situation where the family of functions is parameterized by a subset of $\mathbb{R}^d$, that is, $\mathcal{F}=\{f_\theta,\theta\in\Theta\}$ for $\Theta\subset\mathbb{R}^d$. This includes neural networks and the simplest case of linear model of the form $f_\theta(x)=\theta^T\varphi(x)$, for a certain feature vector $\varphi(x)$.

3.2 Approximation Error

Bounding the approximation error corresponds to bounding $\inf_{f\in\mathcal{F}}\mathcal{R}(f)-\mathcal{R}^*$ and requires assumptions on the Bayes predictor f^* to achieve non-trival learning rates.

Here we will focus on $\mathcal{F}=\{f_\theta,\theta\in\Theta\}$ for $\Theta\subset\mathbb{R}^d$ and a convex Lipschitz-continuous losses. By assuming that θ_* is the minimizer of $\mathcal{R}(f_\theta)$ over $\theta\in\mathbb{R}^d$ (typically, it does not need to belong to Θ), the approximation error decomposes into

$$\inf_{\theta\in\Theta}\mathcal{R}(f_\theta)-\mathcal{R}^*=\left(\inf_{\theta\in\Theta}\mathcal{R}(f_\theta)-\inf_{\theta\in\mathbb{R}^d}\mathcal{R}(f_\theta)\right)+\left(\inf_{\theta\in\mathbb{R}^d}\mathcal{R}(f_\theta)-\mathcal{R}^*\right) \tag{3.2}$$

The second term $\inf_{\theta\in\mathbb{R}^d}\mathcal{R}(f_\theta)-\mathcal{R}^*$ is an incompressible error coming from the chosen of hypothesis space $\mathcal{F}$. While the first term $\theta\mapsto\mathcal{R}(f_\theta)-\inf_{\theta\in\mathbb{R}^d}\mathcal{R}(f_\theta)$ is positive on $\mathbb{R}^d$, which can be typically upperbounded by a certain norm $\Omega(\theta-\theta_*)$. Hence it represents a distance between minimizer θ_* and set Θ on $\mathbb{R}$

For example, if the loss $l(y,\hat{y})$ which is considered as G-Lipschitz-continuous with respect to the second

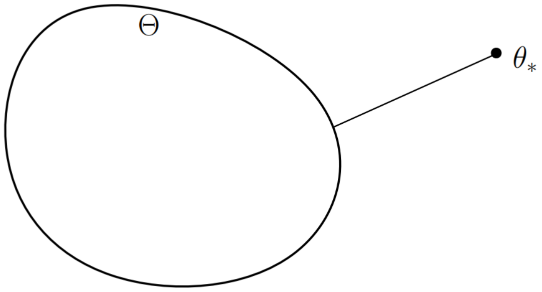


Figure 5: The distance between minimizer θ_* and set Θ on $\mathbb{R}$

variable $\hat{y}$ (possible for regression or convex surrogate for binary classification), we have

$$\mathcal{R}(f_\theta) - \mathcal{R}(f_{\theta'}) = \mathbb{E}\Big[l\big(Y, f_\theta(X)\big) - l\big(Y, f_{\theta'}(X)\big)\Big] \le G \cdot \mathbb{E}\big[|f_\theta(X) - f_{\theta'}(X)|\big]$$

and hence the first term is upper bounded by G times the smallest distance between f_{θ_*} and $\mathcal{F} = \{f_\theta, \theta \in \Theta\}$. A classical example will be $f_\theta(x) = \theta^T \varphi(x)$, and $\Theta = \{\theta \in \mathbb{R}^d, ||\theta||_2 \le D\}$, leading to the upper bound

$$\inf_{\theta\in\Theta} \mathcal{R}(f_\theta) - \inf_{\theta\in\mathbb{R}^d} \mathcal{R}(f_\theta) \le G \cdot \mathbb{E}\big[||\varphi(x)||_2\big]\big(||\theta_*||_2 - D\big)^+$$

which is equalt zero if $||\theta_*||_2 \le D$.

3.3 Estimation Error

The estimation error is often decomposed using the minimizer of the expected risk for our class of models $\mathcal{F}$, $g \in \arg\min_{g\in\mathcal{F}} \mathcal{R}(g)$; and the minimizer of the empirical risk, $\hat{f} \in \arg\min_{f\in\mathcal{F}} \hat{\mathcal{R}}(f)$. That is

$$\begin{aligned} \mathcal{R}(\hat{f}) - \inf_{f\in\mathcal{F}} \mathcal{R}(f) = \mathcal{R}(\hat{f}) - \mathcal{R}(g) &= \Big\{\mathcal{R}(\hat{f}) - \hat{\mathcal{R}}(\hat{f})\Big\} + \Big\{\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(g)\Big\} + \Big\{\hat{\mathcal{R}}(g) - \mathcal{R}(g)\Big\} \\ &\le \sup_{f\in\mathcal{F}} \Big\{\mathcal{R}(f) - \hat{\mathcal{R}}(f)\Big\} + \Big\{\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(g)\Big\} + \sup_{f\in\mathcal{F}} \Big\{\hat{\mathcal{R}}(f) - \mathcal{R}(f)\Big\} \\ &\le \sup_{f\in\mathcal{F}} \Big\{\mathcal{R}(f) - \hat{\mathcal{R}}(f)\Big\} + 0 + \sup_{f\in\mathcal{F}} \Big\{\hat{\mathcal{R}}(f) - \mathcal{R}(f)\Big\} \\ &\le 2 \sup_{f\in\mathcal{F}} \Big|\hat{\mathcal{R}}(f) - \mathcal{R}(f)\Big| \end{aligned} \tag{3.3}$$

The inequality in the third row holds because we assume $\hat{f}$ is the minimizer of empirical risk, so we have $\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}} \le 0$. When $\hat{f}$ is not the global minimizer of $\hat{\mathcal{R}}$ but simply satisfies $\hat{\mathcal{R}}(\hat{f}) \le \inf_{f\in\mathcal{F}} \hat{\mathcal{R}}(f) + \varepsilon$, then the *optimization error* ε has to be added to the bound above

In general, there are two ways to bound the supremum of empirical process $\sup_{f\in\mathcal{F}} \Big|\hat{\mathcal{R}}(f) - \mathcal{R}(f)\Big|$.

- Directly bound $\sup_{f\in\mathcal{F}} |\hat{\mathcal{R}}(f) - \mathcal{R}(f)|$ with high probability (note that $\hat{\mathcal{R}}(f)$ here is a random variable, so we can bound it with high probability)
- Bound the uniform deviaiton of $\sup_{f\in\mathcal{F}} |\hat{\mathcal{R}}(f) - \mathcal{R}(f)|$ from its expectation; and then bound the expectation $\mathbb{E}[\sup_{f\in\mathcal{F}} |\hat{\mathcal{R}}(f) - \mathcal{R}(f)|]$

Before we go deep into the theory of uniform convergence, we see some simple examples.

3.3.1 Uniform Deviation from Expectation

Let

$$H(Z_1, \dots, Z_n) = \sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\}$$

where the random variables $z_i = (x_i, y_i)$ are independent and identically distributed, and $\hat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^{n} l(Y_i, f(X_i))$. We let l_∞ be the maximal absolute value of the loss functions for all (X, Y) in the support of the data generating distribution and $f \in \mathcal{F}$, that is $l_\infty = \max_i |l(Y_i, f(X_i))|$.

When changing a single $Z_i \in \mathcal{X} \times \mathcal{Y}$ into $Z_i' \in \mathcal{X} \times \mathcal{Y}$, the bounded difference of H is almost surely at most $\frac{2}{n} l_\infty$, that is because

$$\begin{aligned}
\left|H(Z_1, \dots, Z_i, \dots, Z_n) - H(Z_1, \dots, Z_i', \dots Z_n)\right| &= \left| \sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\} - \sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}'(f) - \mathcal{R}'(f) \right\} \right| \\
&\leq \left| \sup_{f \in \mathcal{F}} \hat{\mathcal{R}}(f) - \sup_{f \in \mathcal{F}} \hat{\mathcal{R}}'(f) \right| \\
&\leq \left| \sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \hat{\mathcal{R}}'(f) \right\} \right| \\
&= \left| \sup_{f \in \mathcal{F}} \left\{ \frac{1}{n} (l(Z_i) - l(Z_i')) \right\} \right| \leq \frac{2}{n} l_\infty
\end{aligned}$$

where the third inequality holds beacue in general, $\sup_h A(f) - \sup_f B(f) \leq \sup_f [A(f) - B(f)]$. Now, we can apply the MacDiarmid inequality,

$$\mathbb{P}\Big(H(Z_1, \dots, Z_n) - \mathbb{E}[H(Z_1, \dots, Z_n)] \geq t \Big) \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^{n} (\frac{2}{n} l_\infty)^2} \right) = \exp\left(-\frac{nt^2}{2l_\infty^2} \right)$$

By setting $\delta = \exp\left(-nt^2/2l_\infty^2\right)$, which leads to $t = l_\infty \sqrt{\frac{2\log(1/\delta)}{n}}$, with probability greater than $1 - \delta$, we have

$$H(Z_1, \dots, Z_n) - \mathbb{E}[H(Z_1, \dots, Z_n)] \leq l_\infty \sqrt{\frac{2\log(1/\delta)}{n}}$$

Therefore, recall that $H(Z_1, \dots, Z_n) = \sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\}$, we have

$$\sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\} \leq l_\infty \sqrt{\frac{2\log(1/\delta)}{n}} + \mathbb{E}_{S_n} \left[\sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\} \right] \tag{3.4}$$

where $\hat{\mathcal{R}}(f)$ is a random variable relying on training samples S_n. We thus only need to bound the expectation of $\sup_{f \in \mathcal{F}} \left\{ \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right\}$, and add on top of the above result.

3.3.2 Linear Hypothesis Space

In this case, we consider the case when the hypothesis function space $\mathcal{F} = \{\theta^\top \varphi(x) \mid ||\theta||_2 \leq D\}$ is linear with l_2-ball constraint (l_2-norm bounded by D), and the loss function is quadratic, that is

$$l(Y, f(X)) = (Y - \theta^\top \varphi(X))^2$$

From these we get

$$\hat{\mathcal{R}}(f) - \mathcal{R}(f) = \theta^\top \left(\frac{1}{n} \sum_{i=1}^{n} \varphi(X_i)\varphi(X_i)^\top - \mathbb{E}[\varphi(X)\varphi(X)^\top] \right) \theta \\ - 2\theta^\top \left(\frac{1}{n} \sum_{i=1}^{n} Y_i \varphi(X_i) - \mathbb{E}[Y\varphi(X)] \right) + \left(\frac{1}{n} \sum_{i=1}^{n} Y_i^2 - \mathbb{E}[Y^2] \right)$$

Hence, the supremum can be upper bounded in closed from as

$$\sup_{||\theta||_2 \leq D} |\hat{\mathcal{R}}(f) - \mathcal{R}(f)| \leq D^2 \left\| \frac{1}{n} \sum_{i=1}^{n} \varphi(X_i)\varphi(X_i)^\top - \mathbb{E}[\varphi(X)\varphi(X)^\top] \right\|_{op} \\ + 2D \left\| \frac{1}{n} \sum_{i=1}^{n} Y_i \varphi(X_i) - \mathbb{E}[Y\varphi(X)] \right\|_2 + \left| \frac{1}{n} \sum_{i=1}^{n} Y_i^2 - \mathbb{E}[Y^2] \right|$$

where $||M||_{op}$ is the operator norm of the matrix M defined as $||M||_{op} = \sup_{||u||_2=1} ||Mu||_2$.

- Bounding the Matrix

  Suppose $\varphi(\cdot)$ is a d-dimensional function of X. Let

  $$M_i = \varphi(X_i)\varphi(X_i)^\top - \mathbb{E}[\varphi(X)\varphi(X)^\top]$$

  Then M_i is a $d \times d$ symmetric matrix with $\mathbb{E}[M_i = 0]$. Given a sequence of n i.i.d symmetric matricies $\{M_i,\ i = 1, \ldots, n\}$, we can apply matrix Hoeffding's inequality and get

  $$\mathbb{P}\left(\lambda_{\max} \left(\frac{1}{n} \sum_{i=1}^{n} M_i \right) \geq t \right) \leq d \cdot \exp\left(-\frac{nt^2}{8\sigma^2} \right)$$

  where $\sigma^2 = \lambda_{\max}(\bar{M})$. With probability $1 - \delta$, we have $t = \sigma\sqrt{\frac{8\log(d/\delta)}{n}}$ and

  $$\lambda_{\max} \left(\frac{1}{n} \sum_{i=1}^{n} M_i \right) \leq \sigma \sqrt{\frac{8\log(d/\delta)}{n}}$$

  Notice that $\bar{M} = (\frac{1}{n}\sum_{i=1}^{n} M_i)$ is also a symmetric matrix, for any vector θ, we have

  $$\theta^T \left(\frac{1}{n} \sum_{i=1}^{n} M_i \right) \theta \leq \lambda_{\max} \left(\frac{1}{n} \sum_{i=1}^{n} M_i \right) \theta^T\theta \leq D^2 \sigma \sqrt{\frac{8\log(d/\delta)}{n}}$$

- Bounding the Vector

Suppose $\varphi(X)$ is a d-dimensional vector, then we're going to find a uniform bound for its l_2-norm.

$$\begin{aligned}
\mathbb{P}\left(\left\|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi(X_i)-\mathbb{E}[Y_i\varphi(X_i)]\right\|_2\geq t\right) &= \mathbb{P}\left(\left[\sum_{j=1}^{d}\left|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi_j(X_i)-\mathbb{E}[Y_i\varphi_j(X_i)]\right|^2\right]^{1/2}\geq t\right)\\
&= \mathbb{P}\left(\sum_{j=1}^{d}\left|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi_j(X_i)-\mathbb{E}[Y_i\varphi_j(X_i)]\right|^2\geq t^2\right)\\
&\leq \sum_{j=1}^{d}\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi_j(X_i)-\mathbb{E}[Y_i\varphi_j(X_i)]\right|^2\geq \frac{t^2}{d}\right) \quad \text{(union bound)}\\
&= \sum_{j=1}^{d}\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi_j(X_i)-\mathbb{E}[Y_i\varphi_j(X_i)]\right|\geq \frac{t}{\sqrt{d}}\right)
\end{aligned}$$

Now, if we assume $|Y\varphi_j(X)|$ are uniformly bounded by constant c for any $j\in\{1,\ldots,d\}$, we can apply Hoeffding's inequality and get

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi_j(X_i)-\mathbb{E}[Y_i\varphi_j(X_i)]\right|\geq t\right)\leq 2\exp\left(-\frac{2nt^2}{dc^2}\right)$$

which leads to the fact that

$$\mathbb{P}\left(\left\|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi(X_i)-\mathbb{E}[Y_i\varphi(X_i)]\right\|_2\geq t\right)\leq\sum_{j=1}^{d}2\exp\left(-\frac{2nt^2}{dc^2}\right)=2d\exp\left(-\frac{2nt^2}{dc^2}\right) \tag{3.5}$$

Finally, with probability $1-\delta$, we have

$$\left\|\frac{1}{n}\sum_{i=1}^{n}Y_i\varphi(X_i)-\mathbb{E}[Y_i\varphi(X_i)]\right\|_2\leq c\sqrt{\frac{d\log(2d/\delta)}{2n}}$$

- Bouding the Scalar

  Similarily, suppose $Z=Y^2$ is a bounded variable with support $[a,b]$, then applying the Hoeffding's bound, we have with probability $1-\delta$

$$\left|\frac{1}{n}\sum_{i=1}^{n}Y_i^2-\mathbb{E}[Y^2]\right|\leq(b-a)\sqrt{\frac{\log(2/\delta)}{2n}}$$

Finally, by letting $\delta'=\delta/3$ in each of the three bounds above and applying union bound again, we can upper-bond the empirical process with probability $1-\delta$,

$$\begin{aligned}
\sup_{||\theta||_2\leq D}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)| &\leq D^2\sigma\sqrt{\frac{8\log(3d/\delta)}{n}}+2Dc\sqrt{\frac{\log(6d/\delta)}{2n}}+(b-a)\sqrt{\frac{\log(6/\delta)}{2n}}\\
&\approx(4D^2\sigma+2Dc+b-a)\sqrt{\frac{\log(6/\delta)}{2n}}=\mathcal{O}\left(\frac{1}{n}\right)
\end{aligned}$$

3.3.3 Finite Hypothesis Space

We assume in this section that the loss functions $l(Y,f(X))$ are bounded between $-l_\infty$ and l_∞.

Direct Bounding Approach. Using the upper-bound $2\sup_{f\in\mathcal{F}}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|$ on the estimation error, we have the union bound:

$$\mathbb{P}\left(\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\geq t\right)\leq\mathbb{P}\left(2\sup_{f\in\mathcal{F}}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|\geq t\right)\leq\sum_{f\in\mathcal{F}}\mathbb{P}\left(2\left|\hat{\mathcal{R}}(f)-\mathcal{R}(f)\right|\geq t\right)$$

We have, for $f\in\mathcal{F}$ fixed, $\hat{\mathcal{R}}(f)=\frac{1}{n}\sum_{i=1}^{n}l(Y_i,f(X_i))$ and we can apply Hoeffding's inequality to bound each $\mathbb{P}\left(2|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|\geq t\right)$, leading to

$$\mathbb{P}\left(\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\geq t\right)\leq\sum_{f\in\mathcal{F}}2\exp\left(-\frac{nt^2}{2l_\infty^2}\right)=2|\mathcal{F}|\exp\left(-\frac{nt^2}{2l_\infty^2}\right)$$

Thus, by setting $\delta=2|\mathcal{F}|\exp\left(-nt^2/2l_\infty^2\right)$, and finding the corresponding t, with probability greater than $1-\delta$,

$$\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\leq 2l_\infty\sqrt{\frac{\log(2|\mathcal{F}|/\delta)}{n}}\tag{3.6}$$

Bounding the Expectation. In terms of expectation, we get (using the proof of the expectation of the maximum, which apply both bounded and sub-Gaussian random variables)

$$\mathbb{E}\left[\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\right]\leq 2\mathbb{E}\left[\sup_{f\in\mathcal{F}}\left|\hat{R}(f)-\mathcal{R}(f)\right|\right]\leq 2l_\infty\sqrt{\frac{2\log|\mathcal{F}|}{n}}\tag{3.7}$$

Here is the proof, when function family $\mathcal{F}$ is finite, we have

$$\begin{aligned}\mathbb{E}\left[\sup_{f\in\mathcal{F}}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|\right]&=\mathbb{E}\left[\max\left\{\hat{R}(f_1)-\mathcal{R}(f),\ldots,\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\hat{\mathcal{R}}(f_{|\mathcal{F}|})\right\}\right]\\&=\mathbb{E}\left[\frac{1}{n}\log e^{t\max\left\{\hat{R}(f_1)-\mathcal{R}(f),\ldots,\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\hat{\mathcal{R}}(f_{|\mathcal{F}|})\right\}}\right]\\&\leq\frac{1}{t}\log\mathbb{E}\left[e^{t\max\left\{\hat{R}(f_1)-\mathcal{R}(f),\ldots,\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\hat{\mathcal{R}}(f_{|\mathcal{F}|})\right\}}\right]\quad\text{(Jensen's Inequality)}\\&=\frac{1}{t}\log\mathbb{E}\left[\max\left\{e^{t(\hat{\mathcal{R}}(f_1)-\mathcal{R}(f_1))}+\cdots+e^{t(\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\mathcal{R}(f_{|\mathcal{F}|}))}\right\}\right]\\&\leq\frac{1}{t}\log\mathbb{E}\left[e^{t(\hat{\mathcal{R}}(f_1)-\mathcal{R}(f_1))}+\cdots+e^{t(\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\mathcal{R}(f_{|\mathcal{F}|}))}\right]\quad\text{(bounding the max by the sum)}\end{aligned}$$

Since the Chernoff bound of bounded loss $l(Y,f(X))$ is

$$\begin{aligned}\mathbb{E}\left[e^{t(\hat{\mathcal{R}}(f_k)-\mathcal{R}(f_k))}\right]&=\prod_{i=1}^{n}\mathbb{E}\left[e^{\frac{t}{n}(l(Y_i,f_k(X_i))-\mathbb{E}[l(Y_i,f_k(X_i))])}\right]\\&\leq\prod_{i=1}^{n}\exp\left(\frac{l_\infty^2t^2}{2n^2}\right)=\exp\left(\frac{l_\infty^2t^2}{2n}\right)\end{aligned}$$

Substitute the result back to the expectation of estimation error, we get

$$\begin{aligned}\mathbb{E}\left[\sup_{f\in\mathcal{F}}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|\right] &\leq \frac{1}{t}\log\mathbb{E}\left[e^{t(\hat{\mathcal{R}}(f_1)-\mathcal{R}(f_1))}+\cdots+e^{t(\hat{\mathcal{R}}(f_{|\mathcal{F}|})-\mathcal{R}(f_{|\mathcal{F}|}))}\right]\\ &\leq \frac{1}{t}\log\left(|\mathcal{F}|\exp\left(\frac{l_\infty^2 t^2}{2n}\right)\right)\\ &= \frac{\log|\mathcal{F}|}{t}+l_\infty^2\frac{t}{2n}\end{aligned}$$

Minimizer over t, we get $t=\frac{\sqrt{2n\log|\mathcal{F}|}}{l_\infty}$, and therefore

$$\mathbb{E}\left[\sup_{f\in\mathcal{F}}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)|\right]\leq l_\infty\sqrt{\frac{2\log|\mathcal{F}|}{n}}$$

Finaly, plugging the above result into the equation 3.4, we have with probabaility $1-\delta$

$$\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\leq 2\sup_{f\in\mathcal{F}}\left\{\hat{\mathcal{R}}(f)-\mathcal{R}(f)\right\}\leq 2l_\infty\left(\sqrt{\frac{2\log(1/\delta)}{n}}+\sqrt{\frac{2\log|\mathcal{F}|}{n}}\right) \tag{3.8}$$

3.3.4 Beyond the Finite Hypothesis Space

The simple idea behind covering numbers is to deal with function spaces (with infinitely many elements by approximating them through a finite numner of elements. This is often refered to as an "ε-net argument".

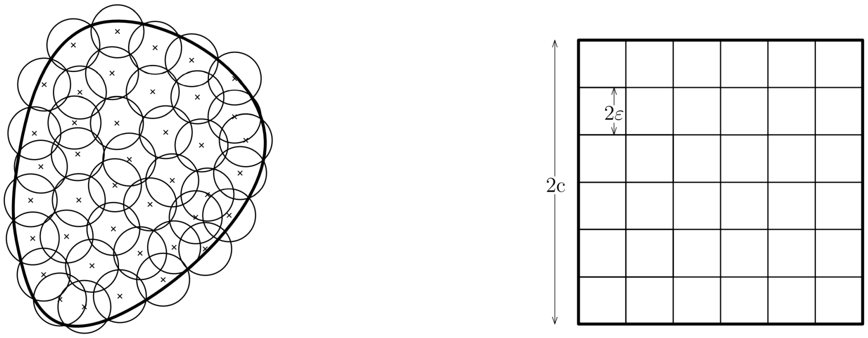


Figure 6: The left picture is an example in two dimensions of a covering with Euclidean balls; The right is an example of l_∞-balls

Definition 3.1 (Covering Numbers)**.** We assume there exists $m=m(\varepsilon)$ elements $f_1,\ldots,f_m$ such that for any $f\in\mathcal{F}$, there exists $i\in\{1,\ldots,n\}$ such that $d(f,f_i)\leq\varepsilon$. The minimal possible number $m(\varepsilon)$ is the covering number of $\mathcal{F}$ at precision ε.

We first need to assume that the risks $\mathcal{R}$ and $\hat{\mathcal{R}}$ are regular, for example, they are G-Lipschitz-continuous with respect to some distance d on $\mathcal{F}$. Now, given a cover of $\mathcal{F}$, for all $f\in\mathcal{F}$, and with $(f_i)_{i\in\{1,\ldots,m_\varepsilon\}}$ the associated cover elements

$$\begin{aligned}|\hat{\mathcal{R}}(f)-\mathcal{R}(f)| &\leq |\hat{\mathcal{R}}(f)-\hat{\mathcal{R}}(f_i)|+|\hat{\mathcal{R}}(f_i)-\mathcal{R}(f_i)|+|\mathcal{R}(f_i)-\mathcal{R}(f)|\\ &\leq 2G\varepsilon+\sup_{i\in\{1,\ldots,m(\varepsilon)\}}|\hat{\mathcal{R}}(f_i)-\mathcal{R}(f_i)|\end{aligned}$$

Using bounds 3.7 on the expectation of the maximum (bounded random variables are sub-Gaussian), we have

$$\begin{aligned} \mathbb{E}\left[\sup_{f\in\mathcal{F}}\left|\hat{\mathcal{R}}(f)-\mathcal{R}(f)\right|\right] &\leq 2G\varepsilon+\mathbb{E}\left[\sup_{i\in\{1,\ldots,m(\varepsilon)\}}\left|\hat{\mathcal{R}}(f_i)-\mathcal{R}(f_i)\right|\right] \\ &\leq 2G\varepsilon+l_\infty\sqrt{\frac{2\log m(\varepsilon)}{n}} \end{aligned} \tag{3.9}$$

The first term of the bound capture the estmation biased controlled by ε, while the second tem characterize the complexity of the covering.

- Therefore, if $m(\varepsilon)\sim\varepsilon^{-d}$, ignoring constants, we need to balance $\varepsilon+\sqrt{\frac{d\log(1/\varepsilon)}{n}}$, which leads to, with a choice of ε proportional to $1/\sqrt{n}$, to a rate proportional $\sqrt{\frac{d\log n}{n}}$
- Unfortunately, this often leads to a non-optimal dependence on sample size n (because of the existence of $\log n$), as the rate is essentially proportional to $\sqrt{d/n}$
- One very powerful tool that avoids these undesired dependences on dimension is Rademacher complexities or Gaussian complexities

4 PAC Learning and Uniform Convergence

4.1 PAC Learning

In the previous section, we have shown that for a finite hypothesis space, if the ERM rule with respect to that class is applied on a sufficiently large training sample (whose size is independent of the underlying distribution or labeling function) then the output hypothesis will be probably approximately correct. More generally, we now define *Probably Approximately Correct* (PAC) learning.

Definition 4.1 (PAC Learnability)**.** A hypothesis class $\mathcal{F}$ is PAC learnable if there exist a function $m_{\mathcal{F}} : (0,1)^2 \mapsto \mathbb{N}$ and a learning algorithm with the following property: for every $\varepsilon, \delta \in (0,1)$ and for every probability distribution P over $\mathcal{X}$, and for every labeling function $g : \mathcal{X} \mapsto \{0,1\}$, if the realizable assumption holds with respect to $\mathcal{F}, P, g$, then when running the learning algorithm on $m \geq m_{\mathcal{F}}(\varepsilon, \delta)$ i.i.d examples generated by P and labeled by g, the algorithms returns a hypothesis f, such that, with probability of at least $1 - \delta$,

$$\mathcal{R}_{P,g}(f) \leq \varepsilon$$

where $\mathcal{R}_{P,g}(f) = \mathbb{E}_P[l(g(X), f(X))]$ and $l(y, \hat{y})$ is a loss function.

The definition of Probably Approximately Correct learnability contains two approximation parameters:

- the accuracy parameter ε determines how far the output classifier can be from the optimal one (approximately correct)
- and the confidence parameter δ indicating how likely the classifier is to meet the accuracy requriement (probably)

Sample Complexity. The function $m_{\mathcal{F}} : (0,1)^2 \mapsto \mathbb{N}$ determines the *sample complexity* of learning $\mathcal{F}$: that is, how many examples are required to guarantee a probably approximately correct solution. The sample complexity $m_{\mathcal{F}}$ is a function of accuracy (ε) and confidence (δ) parameters. It also depends on properties of the hypothesis class $\mathcal{F}$ – for example, for a finite class we showed that the sample comolexity depends on log the size of $\mathcal{F}$ (see Section 3.3.3).

Note that if $\mathcal{F}$ is PAC learnable, there are many functions $m_{\mathcal{F}}$ that satisfy the requirement given in the definition of PAC learnability. Therefore, to be precise, we will define the sample complexity of learning $\mathcal{F}$ to be the ”minimal function”, in the sense that for any (ε, δ), $m_{\mathcal{F}}(\varepsilon, \delta)$ is the minimal integer that satisfies the requirements of PAC learning.

Corollary 4.1. Every finite hypothesis class is PAC learnable with sample complexity

$$m_{\mathcal{F}}(\varepsilon, \delta) \leq \left\lceil \frac{\log(|\mathcal{F}|/\delta)}{\varepsilon} \right\rceil$$

There are infinite classes that are learnable as well. Later on we will show that what determines the PAC learnability of a class is not its finiteness but rather a combinatorial measure called the *VC dimension.*

4.2 Agnostic PAC Learning

The model we have just described can be readily generalized, so that it can be made relevant to a wide scope of learning tasks. We consider generalizations in two aspects:

- Relaxing the realizability assumption

- Learning problems beyond binary classification

Definition 4.2 (Agnostic PAC Learnability)**.** A hypothesis class $\mathcal{F}$ is agnostic PAC learnable if there exist a function $m_{\mathcal{F}} : (0,1)^3 \mapsto \mathbb{N}$ and a learning algorithm with the following property: for every $\varepsilon, \delta \in (0,1)$ and for every distribution S_n over $\mathcal{X} \times \mathcal{Y}$, when running the learning algorithm on $m \geq m_{\mathcal{F}}(\varepsilon, \delta)$ i.i.d. examples generated by probability distribution P, the algorithm returns a hypothesis h such that, with probability of at least $1 - \delta$ (over the choice of the m training examples),

$$\mathcal{R}(f) - \inf_{f' \in \mathcal{F}} \mathcal{R}(f') \leq \varepsilon$$

where here we simply denote $\mathcal{R} = \mathcal{R}_P$ as the expected risk.

4.3 Uniform Convergence

In this section, we will show that uniform convergence is sufficient for learnability. The idea behind the learning condition discussed here is very simple. Recall that, given a hypothesis class, $\mathcal{F}$, the empirical risk minimization (ERM) learning a paradigm works as follows: Uppon recieving a training sample S, the learner evaluates the risk of each f in $\mathcal{F}$ on the given sample and outputs a member of $\mathcal{F}$ that minimizes this empirical risk.

The hope is that an f minimizes the empirical risk with respect to S is a risk minimizer (or has risk close to the minimum) with respect to the true data probability distribution P as well. Recall that we have shown previously that

$$\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \leq 2 \sup_{f \in \mathcal{F}} \left| \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right| \tag{4.1}$$

Hence, for that, it suffices to ensure that the empirical risks of all members of $\mathcal{F}$ are good approximations of their true risk. Put another way, we need that uniformly over all hypotheses in the hypothesis class, the empirical risk will be close to the true risk, as formalized in the following.

Definition 4.3 (ε-representative sample)**.** A training set S is called ε-representative (w.r.t. domain $\mathcal{X}$, distribution P, hypothesis class $\mathcal{F}$ and loss function l) if

$$\forall\, f \in \mathcal{F}, \; \left| \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right| \leq \varepsilon$$

where here we dentoe $\hat{\mathcal{R}} = \mathcal{R}_S$ as the empirical risk with respect to sample S and $\mathcal{R} = \mathcal{R}_P$ the expected risk.

The next simple lemma states that whenever the sample is $\varepsilon/2$-representative, the ERM leanring rule is guaranteed to return a good hypothesis.

Lemma 4.2. Assume that a training set S is $\varepsilon/2$-representative (w.r.t. domain $\mathcal{X}$, distribution P, hypothesis class $\mathcal{F}$ and loss function l). Then, any output of $\mathrm{ERM}_{\mathcal{R}}(S)$, namely, any $\hat{f} \in \arg\min_{f \in \mathcal{F}} \hat{R}(f)$, satisifies

$$\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \leq \varepsilon$$

Proof. From Eq.(4.1), we know that

$$\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \leq 2 \sup_{f \in \mathcal{F}} \left| \hat{\mathcal{R}}(f) - \mathcal{R}(f) \right|$$

Since the training sample S is $\varepsilon/2$-representative, namely, $|\hat{\mathcal{R}}(f) - \mathcal{R}(f)| \leq \varepsilon/2$, we have

$$\mathcal{R}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \leq \varepsilon$$

□

The preceding lemma implies that to ensure that the **ERM is an agnostic PAC learner**, it suffices to show that with probability of at least $1 - \delta$ over the random choice of a training set, it will be an ε-representative training set. The uniform convergence condition formalizes this requirement.

Definition 4.4 (Uniform Convergence)**.** We say that a hypothesis class $\mathcal{F}$ has the uniform convergence property (w.r.t. a domain $\mathcal{X}$ and a loss function l) if there exists a function

$$m_{\mathcal{F}}^{\mathrm{UC}} : (0,1)^2 \mapsto \mathbb{N}$$

such that for every $\varepsilon, \delta \in (0,1)$ and for every probability distribution P over $\mathcal{X}$, if $\mathcal{S}$ is a sample of $m \geq m_{\mathcal{F}}^{\mathrm{UC}}(\varepsilon, \delta)$ examples drawn i.i.d from P, then, with probability of at least $1 - \delta$, sample $\mathcal{S}$ is ε-represnetative.

Similar to the definition of sample complexity for PAC learning, the function $m_{\mathcal{F}}^{\mathrm{UC}}$ measures the (minimal) sample complexity of obtaining the uniform convergence property, namely, how many examples we need to ensure that with probability of at least $1 - \delta$ the sample would be ε-representative.

Remark 4.1. The term *uniform* here refers to having a fixed sample size that works for all members of $\mathcal{F}$ and for all possible probability distributions P over the domain and some loss function.

Corollary 4.3. If a class $\mathcal{F}$ has the uniform convergence property with a function $m_{\mathcal{F}}^{UC}$ then the class is agnostically PAC learnable with the sample complexity $m_{\mathcal{F}}(\varepsilon, \delta) \leq m_{\mathcal{F}}^{UC}(\varepsilon/2, \delta)$. Furthermore, in that case, the $\mathrm{ERM}_{\mathcal{F}}$ paradigm is a successful agnostic PAC learner for $\mathcal{F}$.

5 Rademacher Complexity

In Section 4 we have shown that uniform convergence is a sufficient condition for learnability. In this section, we study the Rademacher complexity, which measures the rate of uniform convergence. We will provide generailization bounds based on this measure. To begin with, let's recall the definition of an ε-representative sample.

5.1 Motivation for Rademacher Complexity

Definition 5.1 (ε-representative sample)**.** A training set S is called ε-representative (w.r.t. domain $\mathcal{X}$, distribution P, hypothesis class $\mathcal{F}$ and loss function l) if

$$\sup_{f\in\mathcal{F}}\left|\hat{\mathcal{R}}(f)-\mathcal{R}(f)\right|\leq\varepsilon$$

From Eq.(4.1) we know that if S is an $\varepsilon/2$-representative sample set, then the empirical risk minimization (ERM) rule is ε-consistent, namely, $\mathcal{R}(\hat{f})-\inf_{f\in\mathcal{F}}\mathcal{R}(f)\leq\varepsilon$, where $\hat{f}=\mathrm{ERM}_{\mathcal{F}}(S)$. For simplicity, we define a new variable Z over domain $\mathcal{Z}=\mathcal{X}\times\mathcal{Y}$, and a function h from hypothesis space $\mathcal{H}=\{h:(Y,X)\mapsto l(Y,f(X))\mid f\in\mathcal{F}\}$. The expected risk (w.r.t. probability distribution P) and the empirical risk (w.r.t. some sample set) are defined as follows:

$$\mathcal{R}(h)=\mathbb{E}[h(Z)]\quad\text{and}\quad\hat{\mathcal{R}}(h)=\frac{1}{n}\sum_{S}h(Z)$$

We define the *representativeness* of S with respect to $\mathcal{H}$ as the largest gap between the expected risk of a function h and its empirical risk, that is,

$$\mathrm{Rep}_P(\mathcal{H},S):=\sup_{h\in\mathcal{H}}\hat{R}(h)-\mathcal{R}(h)\tag{5.1}$$

Now suppose we would like to estimate the representativeness of S using the sample S only. One simple idea is to split S into two disjionit sets, $S=S_1\cup S_2$; refer S_1 as a training set and to S_2 as a validation set. We can then estimate the representativeness of S by

$$\sup_{h\in\mathcal{H}}\ \hat{\mathcal{R}}_{S_1}(h)-\hat{\mathcal{R}}_{S_2}(h)\tag{5.2}$$

This can be written more compactly by defining $\sigma=(\sigma_1,\ldots,\sigma)\in\{\pm1\}^n$ to be a vector such that $S_1=\{Z_i:\sigma_i=1\}$ and $S_2=\{Z_i:\sigma_i=-1\}$. Then, if we further assume that $|S_1|=|S_2|$, then the equation above can be rewritten as

$$\sup_{h\in\mathcal{H}}\ \frac{2}{n}\sum_{i=1}^{n}\sigma_i h(Z_i)\tag{5.3}$$

The Rademacher complexity measure this idea by considering the expectation of the above with respect to a random choice of Rademacher variable σ. We will see the formal definition in next section.

5.2 Rademacher Complexity

Rememeber that our goal here is to provide an upper-bound on the empirical process $\sup_{f\in\mathcal{F}}\{\hat{\mathcal{R}}(f)-\mathcal{R}(f)\}$ introduced in Section 3.3, which happens to be equal to

$$\sup_{h\in\mathcal{H}}\left\{\frac{1}{n}\sum_{i=1}^{n}h(Z_i)-\mathbb{E}[h(Z)]\right\}$$

Later we will show that the empirical process is upper-bounded by two times the Rademacher complexity. Now, let's see the definition of empirical Rademacher complexity and then the expected Rademacher complexity.

Definition 5.2 (Empirical Rademacher Complexity)**.** Let $\mathcal{H}$ be a family of functions mapping from $\mathcal{Z}$ to $\mathbb{R}$, and $S_n = (Z_1,\ldots,Z_n)$ a fixed sample of size n with elements in $\mathcal{Z}$. Then the empirical Rademacher compelxity of $\mathcal{H}$ with respect to the sample S_n is defined as

$$\hat{R}_{S_n}(\mathcal{H})=\mathbb{E}_\sigma\left[\sup_{h\in\mathcal{H}}\frac{1}{n}\sum_{i=1}^{n}\sigma_i h(Z_i)\right] \tag{5.4}$$

where $\sigma=(\sigma_1,\ldots,\sigma_n)^\top$, with σ_i's independent uniform random variables taking values in $\{\pm1\}$. The random variables σ_i are called Rademacher variables.

Let h_S denote the vector of values taken by function h over the sample S, namely, $h_S=(h(Z_1),\ldots,h(Z_n))^\top$. Then the empirical Rademacher complexity can be rewritten as

$$\hat{R}_{S_n}(\mathcal{H})=\mathbb{E}_\sigma\left[\sup_{h\in\mathcal{H}}\frac{\langle\sigma,h_S\rangle}{n}\right]$$

Thus, the empirical Rademacher complexity measures on average how well the function class $\mathcal{H}$ correlates with random noise on S. This describes the richness of the family $\mathcal{H}$: richer or more complex families $\mathcal{H}$ can generate more vectors h_S and thus better correlate with random noise, on average.

Definition 5.3 (Rademacher Complexity)**.** Let P denote the probability distribution according to which samples are drawn. For any integer $n\geq1$, the Rademacher complexity is the expectation of the empirical Rademahcer complexity over all samples of size n drawn i.i.d. with respect to P.

$$R_n(\mathcal{H})=\mathbb{E}_P\left[\hat{R}_{S_n}(\mathcal{H})\right]=\mathbb{E}_{\sigma,P}\left[\sup_{h\in\mathcal{H}}\frac{1}{n}\sum_{i=1}^{n}\sigma_i h(Z_i)\right] \tag{5.5}$$

Now, we show that, through a general "symmetrization" property, the Rademacher complexity $R_n(\mathcal{H})$ directly controls the expectation of empirical process, that is $\mathbb{E}[\sup_{f\in\mathcal{F}}(\hat{\mathcal{R}}(f)-\mathcal{R}(f))]$.

Theorem 5.1 (Symmetrization)**.** Given the Rademacher complexity of $\mathcal{H}$ defined in equaiton 5.5, we have

$$\mathbb{E}\left[\sup_{h\in\mathcal{H}}\left(\frac{1}{n}\sum_{i=1}^{n}h(Z_i)-\mathbb{E}[h(Z)]\right)\right]\leq 2R_n(\mathcal{H}) \tag{5.6}$$

and

$$\mathbb{E}\left[\sup_{h\in\mathcal{H}}\left(\mathbb{E}[h(Z)]-\frac{1}{n}\sum_{i=1}^{n}h(Z_i)\right)\right]\leq 2R_n(\mathcal{H}) \tag{5.7}$$

Proof. Let $S_n' = \{Z_1', \dots, Z_n'\}$ be an independent copy of the data $S_n = \{Z_1, \dots, Z_n\}$. Let $(\sigma_i)_{i \in \{1,\dots,n\}}$ be i.i.d. Rademacher random variables, which are also independent of S_n and S_n'. Using that for all $i \in \{1, \dots, n\}$, $\mathbb{E}[h(Z_i') \mid S_n] = \mathbb{E}[h(Z)]$, we have

$$\begin{aligned}
\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(Z)] - \frac{1}{n}\sum_{i=1}^n h(Z_i) \right)\right] &= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n \mathbb{E}[h(Z_i') \mid S_n] - \frac{1}{n}\sum_{i=1}^n h(Z_i) \right)\right] \\
&= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n \mathbb{E}[h(Z_i') - h(Z_i) \mid S_n] \right)\right]
\end{aligned}$$

by definition of the independent copy S_n'. Then using that the supremum of the expectation is less than expectation of the supremum,

$$\begin{aligned}
\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(Z)] - \frac{1}{n}\sum_{i=1}^n h(Z_i) \right)\right] &\leq \mathbb{E}\left[\mathbb{E}\left(\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n [h(Z_i') - h(Z_i)] \right) \mid S_n \right)\right] \\
&= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n [h(Z_i') - h(Z_i)] \right)\right] \\
&= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n \sigma_i [h(Z_i') - h(Z_i)] \right)\right] \quad \text{(symmetrization)} \\
&\leq \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n \sigma_i h(Z_i) \right)\right] + \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n -\sigma_i h(Z_i) \right)\right] \\
&= 2\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\frac{1}{n}\sum_{i=1}^n \sigma_i h(Z_i) \right)\right] = 2R_n(\mathcal{H})
\end{aligned}$$

The reasoning is essentially identical for $\mathbb{E}\left[\sup_{h \in \mathcal{H}} \left(\mathbb{E}[h(Z)] - \frac{1}{n}\sum_{i=1}^n h(Z_i) \right)\right] \leq 2R_n(\mathcal{H})$.

□

Theorem 5.2 (Empirical Process bonud via Rademacher Complexity)**.** Suppose for all $h \in \mathcal{H}$, $0 \leq h(Z) \leq 1$. Then, with probability at least $1 - \delta$,

$$\begin{aligned}
\sup_{h \in \mathcal{H}} \left[\frac{1}{n}\sum_{i=1}^n h(Z_i) - \mathbb{E}[h(Z)] \right] &\leq 2R_n(\mathcal{H}) + \sqrt{\frac{\log(2/\delta)}{2n}} \\
\sup_{h \in \mathcal{H}} \left[\frac{1}{n}\sum_{i=1}^n h(Z_i) - \mathbb{E}[h(Z)] \right] &\leq 2\hat{R}_{S_n}(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2n}}
\end{aligned} \tag{5.8}$$

Proof. For conciseness, define

$$H(Z_1, \dots, Z_n) := \sup_{h \in \mathcal{H}} \left[\frac{1}{n}\sum_{i=1}^n h(Z_i) - \mathbb{E}[h(Z_i)] \right]$$

and we prove the theorem for four steps.

- Step 1. We bound H using McDiarmid's inequality. To use McDiarmid's inequality, we firstly check that the bounded difference condition holds:

$$\begin{aligned}
H(Z_1, \ldots, Z_i, \ldots, Z_n) - H(Z_1, \ldots, Z_i', \ldots, Z_n) &\leq \sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{j=1}^{n} h(Z_j) \right\} - \sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{j \neq i}^{n} h(Z_j) + \frac{1}{n} h(Z_i') \right\} \\
&\leq \sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{j=1}^{n} h(Z_j) - \frac{1}{n} \sum_{j \neq i}^{n} h(Z_j) - \frac{h(Z_i')}{n} \right\} \\
&= \sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} (h(Z_i) - H(Z_i')) \right\} \\
&\leq \frac{1}{n} \qquad \text{(given } h(Z) \leq 1\text{)}
\end{aligned}$$

where the second inequality holds beacue in general, $\sup_h A(f) - \sup_f B(f) \leq \sup_f [A(f) - B(f)]$. We can thus apply McDiarmid's inequality with parameters $c_1 = \cdots = c_n = 1/n$,

$$\mathbb{P}\Big(H(Z_1, \ldots, Z_n) - \mathbb{E}[H(Z_1, \ldots, Z_n)] \geq t \Big) \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^n c_i^2} \right) = \exp\left(-2nt^2 \right)$$

that is, with probability $1 - \delta$

$$H(Z_1, \ldots, Z_n) \leq \mathbb{E}[H(Z_1, \ldots, Z_n)] + \sqrt{\frac{\log(2/\delta)}{2n}}$$

where here we set $\exp(-2nt^2) = \delta/2$.

- Step 2. We apply the Theorem 5.1 to get the upper bound of the expectation of the empirical process

  $$\mathbb{E}[H(Z_1, \ldots, Z_n)] \leq 2R_n(\mathcal{H})$$

  which implies

  $$\sup_{h \in \mathcal{H}} \left[\frac{1}{n} \sum_{i=1}^{n} h(Z_i) - \mathbb{E}[h(Z)] \right] \leq 2R_n(\mathcal{H}) + \sqrt{\frac{\log(2/\delta)}{2n}}$$

- Step 3. Bound expected Rademacher complexity through empirical Rademacher complexity and McDiarmid inequality. To begin with, define

  $$\tilde{H} = \hat{R}_{S_n}(\mathcal{H}) := \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i h(Z_i) \right]$$

Using a similar argument in Step 1, we find that $\tilde{H}$ also satisfies the bounded difference condition:

$$\begin{aligned}
\tilde{H}(Z_1, \dots, Z_i, \dots, Z_n) - \tilde{H}(Z_1, \dots, Z_i', \dots, Z_n) &\le \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{j=1}^n h(Z_j) \right\} - \sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{j \neq i}^n h(Z_j) + \frac{1}{n} h(Z_i') \right\} \right] \\
&\le \mathbb{E}\left[\sup_{f \in \mathcal{F}} \left\{ \frac{1}{n} \sum_{j=1}^n h(Z_j) - \frac{1}{n} \sum_{j \neq i}^n h(Z_j) - \frac{h(Z_i')}{n} \right\} \right] \\
&= \mathbb{E}\left[\sup_{h \in \mathcal{H}} \left\{ \frac{1}{n} (h(Z_i) - h(Z_i')) \right\} \right] \\
&\le \frac{1}{n}
\end{aligned}$$

because the term inside the sup is always upper-bounded by 1. We can therefore apply McDiarmid's inequality again with parameter $c_1 = \cdots c_n = 1/n$ and get

$$\mathbb{P}\Big(\tilde{H}(Z_1, \dots, Z_n) - \mathbb{E}[\tilde{H}(Z_1, \dots, Z_n)] \ge t\Big) \le \exp\left(-\frac{2t^2}{\sum_{i=1}^n c_i^2}\right) = \exp\left(-2nt^2\right)$$

and

$$\mathbb{P}\Big(\tilde{H}(Z_1, \dots, Z_n) - \mathbb{E}[\tilde{H}(Z_1, \dots, Z_n)] \le -t\Big) \le \exp\left(-\frac{2t^2}{\sum_{i=1}^n c_i^2}\right) = \exp\left(-2nt^2\right)$$

that is, with probability $1 - \delta$

$$\mathbb{E}[\tilde{H}(Z_1, \dots, Z_n)] \le \tilde{H}(Z_1, \dots, Z_n) + \sqrt{\frac{\log(2/\delta)}{2n}}$$

where here we set $\exp(-2nt^2) = \delta/2$.

- Step 4. Putting all things together by noticing that

$$\mathbb{E}[\tilde{H}] = \mathbb{E}_P[\hat{R}_{S_n}(\mathcal{H})] = R_n(\mathcal{H})$$

we have with probability $1 - \delta$,

$$\begin{aligned}
\sup_{h \in \mathcal{H}} \left[\frac{1}{n} \sum_{i=1}^n h(Z_i) - \mathbb{E}[h(Z)] \right] = H(Z_1, \dots, Z_n) &\le \mathbb{E}[H(Z_1, \dots, Z_n)] + \sqrt{\frac{\log(2/\delta)}{2n}} \qquad \text{(Step 1.)} \\
&\le 2R_n(\mathcal{H}) + \sqrt{\frac{\log(2/\delta)}{2n}} \qquad \text{(Step 2.)} \\
&\le 2\left(\hat{R}_S(\mathcal{H}) + \sqrt{\frac{\log(2/\delta)}{2n}}\right) + \sqrt{\frac{\log(2/\delta)}{2n}} \qquad \text{(Step 3.)} \\
&= 2\hat{R}_S(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2n}}
\end{aligned}$$

□

Corollary 5.3 (Generalization Bonud via Rademacher Complexity). Suppose for all $h \in \mathcal{H}$, $0 \le h(Z) \le 1$.

Then, with probability at least $1 - \delta$,

$$\begin{aligned} \mathbb{E}[h(Z)] &\leq \frac{1}{n}\sum_{i=1}^{n} h(Z_i) + 2R_n(\mathcal{H}) + \sqrt{\frac{\log(2/\delta)}{2n}} \\ \mathbb{E}[h(Z)] &\leq \frac{1}{n}\sum_{i=1}^{n} h(Z_i) + 2\hat{R}_S(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2n}} \end{aligned} \tag{5.9}$$

A useful fact is that both empirical Rademacher complexity and expected Rademacher complexity are translation invariant.

Proposition 5.1 (Translation Invariant)**.** Let $\mathcal{H}$ be a family of functions mapping $\mathcal{Z} \mapsto \mathbb{R}$ and define $\mathcal{H}' = \{h'(Z) = h(Z) + c_0 \mid h \in \mathcal{H}\}$ for some $c_0 \in \mathbb{R}$. Then we have

$$\hat{R}_{S_n}(\mathcal{H}) = \hat{R}_{S_n}(\mathcal{H}') \quad \text{and} \quad R_n(\mathcal{H}) = R_n(\mathcal{H}')$$

Hint. The property of Rademacher random variables. □

5.3 Lipschitz-continuous Losses

A particularly appealing property in our context is the following property, sometimes called the "contraction principle".

Remark 5.1. For a compact intevral, continuously differentiable $\subseteq$ Lipschitz continuous $\subseteq$ absolutely continuous $\subseteq$ bounded variation $\subseteq$ differentiable almost everywhere

Proposition 5.2 (Contraction Principle - Lipschitz-continuous Functions)**.** Given any functions b, $a_i : \Theta \mapsto \mathbb{R}$ (no assumption on Θ) and $\varphi_i : \mathbb{R} \mapsto \mathbb{R}$ any 1-Lipschitz-functions, for $i = 1, \ldots, n$, we have, for $\sigma \in \mathbb{R}^n$ a vector of independent Rademacher random variables,

$$\mathbb{E}_\sigma\left[\sup_{\theta\in\Theta}\ b(\theta) + \sum_{i=1}^{n} \sigma_i \varphi_i(a_i(\theta))\right] \leq \mathbb{E}_\sigma\left[\sup_{\theta\in\Theta}\ b(\theta) + \sum_{i=1}^{n} \sigma_i a_i(\theta)\right] \tag{5.10}$$

Proof. We consider a proof by induction on n. The case $n = 0$ is trivial, and we show how to go from $n \geq 0$ to $n + 1$. We thus consider $\mathbb{E}_{\sigma_1,\ldots,\sigma_{n+1}}\left[\sup_{\theta\in\Theta} b(\theta) + \sum_{i=1}^{n+1} \sigma_i\varphi_i(a_i(\theta))\right]$ and compute the expectation with respect to σ_{n+1} explicitly, by considering the two potential values with probability $1/2$,

$$\begin{aligned} &\mathbb{E}_{\sigma_1,\ldots,\sigma_{n+1}}\left[\sup_{\theta\in\Theta} b(\theta) + \sum_{i=1}^{n+1} \sigma_i\varphi_i(a_i(\theta))\right] \\ =&\frac{1}{2}\mathbb{E}_{\sigma_1,\ldots,\sigma_n}\left[\sup_{\theta\in\Theta} b(\theta) + \sum_{i=1}^{n} \sigma_i\varphi_i(a_i(\theta)) + \varphi_{n+1}(a_{n+1}(\theta))\right] + \frac{1}{2}\mathbb{E}_{\sigma_1,\ldots,\sigma_n}\left[\sup_{\theta\in\Theta} b(\theta) + \sum_{i=1}^{n} \sigma_i\varphi_i(a_i(\theta)) - \varphi_{n+1}(a_{n+1}(\theta))\right] \\ =&\mathbb{E}_{\sigma_1,\ldots,\sigma_n}\left[\sup_{\theta,\theta'\in\Theta} \frac{b(\theta) + b(\theta')}{2} + \sum_{i=1}^{n} \sigma_i \frac{\varphi_i(a_i(\theta)) + \varphi_i(a_i(\theta'))}{2} + \frac{\varphi_{n+1}(a_{n+1}(\theta)) - \varphi_{n+1}(a_{n+1}(\theta'))}{2}\right] \end{aligned}$$

By taking the supremum over (θ, θ') and (θ', θ) and using Lipschitz-continuity, we get

$$\begin{aligned}
&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\left[\sup_{\theta,\theta'\in\Theta}\frac{b(\theta)+b(\theta')}{2}+\sum_{i=1}^n\sigma_i\frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2}+\frac{\varphi_{n+1}(a_{n+1}(\theta))-\varphi_{n+1}(a_{n+1}(\theta'))}{2}\right]\\
=&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\left[\sup_{\theta,\theta'\in\Theta}\frac{b(\theta)+b(\theta')}{2}+\sum_{i=1}^n\sigma_i\frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2}+\frac{\left|\varphi_{n+1}(a_{n+1}(\theta))-\varphi_{n+1}(a_{n+1}(\theta'))\right|}{2}\right]\\
\leq&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\left[\sup_{\theta,\theta'\in\Theta}\frac{b(\theta)+b(\theta')}{2}+\sum_{i=1}^n\sigma_i\frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2}+\frac{\left|a_{n+1}(\theta)-a_{n+1}(\theta')\right|}{2}\right]\\
=&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\left[\sup_{\theta,\theta'\in\Theta}\frac{b(\theta)+b(\theta')}{2}+\sum_{i=1}^n\sigma_i\frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2}+\frac{a_{n+1}(\theta)-a_{n+1}(\theta')}{2}\right]
\end{aligned}$$

The first and last equalities hold becasue of the fact that $\sup_{\theta,\theta'\in\Theta} a_{n+1}(\theta) - a_{n+1}(\theta')$ at least equal to zero. Now, we can redo the exact same sequence of equalities with φ_{n+1} being the identity, to obtain that the last expression above is equal to

$$\begin{aligned}
&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\mathbb{E}_{\sigma_{n+1}}\left[\sup_{\theta\in\Theta}b(\theta)+\sum_{i=1}^n\sigma_i\varphi_i(a_i(\theta))+\sigma_{n+1}a_{n+1}(\theta)\right]\\
\leq&\mathbb{E}_{\sigma_1,\dots,\sigma_n}\mathbb{E}_{\sigma_{n+1}}\left[\sup_{\theta\in\Theta}b(\theta)+\sum_{i=1}^n\sigma_i a_i(\theta)+\sigma_{n+1}a_{n+1}(\theta)\right] \quad \text{by the induction hypothesis}
\end{aligned}$$

which leads to the desired result.

□

We can apply the contraction principle above to supervised learning situations where $u_i \mapsto l(y_i, u_i)$ is G-Lipschitz-continuous for all i almost surely (possible for regression or when using a convex surrogate for binary classification), leading to

$$\mathbb{E}_\sigma\left[\sup_{f\in\mathcal{F}}\frac{1}{n}\sum_{i=1}^n\sigma_i l(Y_i, f(X_i)) \mid S_n\right] \leq G\cdot\mathbb{E}_\sigma\left[\sup_{f\in\mathcal{F}}\frac{1}{n}\sum_{i=1}^n\sigma_i f(X_i) \mid S_n\right] \tag{5.11}$$

by the contraction principle, which leads to

$$\frac{1}{2}\mathbb{E}\left[\sup_{h\in\mathcal{H}}\left(\frac{1}{n}\sum_{i=1}^n\sum_{i=1}^n h(Z_i)-\mathbb{E}[h(Z)]\right)\right] \leq R_n(\mathcal{H}) \leq G\cdot R_n(\mathcal{F}) \tag{5.12}$$

Thus, the Rademacher complexity of the class of prediction functions $R_n(\mathcal{F})$ controls the expectation of empirical process.

5.4 Ball-constrained Linear Predictions

We now assume that $\mathcal{F} = \{f_\theta(X) = \theta^\top\varphi(X) \mid \Omega(\theta) \leq D\}$ where Ω is norm on $\mathbb{R}^d$. We denote by $\Phi \in \mathbb{R}^{n\times d}$ the design matrix, that is,

$$\Phi = \begin{bmatrix}\varphi_1(X_1) & \varphi_2(X_1) & \cdots & \varphi_d(X_1)\\ \varphi_1(X_2) & \varphi_2(X_2) & \cdots & \varphi_d(X_2)\\ \vdots & \vdots & & \vdots\\ \varphi_1(X_n) & \varphi_2(X_n) & \cdots & \varphi_d(X_n)\end{bmatrix}$$

We have

$$\mathcal{R}_n(\mathcal{F}) = \mathbb{E}\left[\sup_{\Omega(\theta)\leq D}\left(\frac{1}{n}\sum_{i=1}^{n}\sigma_i\theta^\top\varphi(X_i)\right)\right] = \mathbb{E}\left[\sup_{\Omega(\theta)\leq D}\left(\frac{1}{n}\sigma^\top\Phi\theta\right)\right] = \frac{D}{n}\mathbb{E}\Big[\Omega^*(\Phi^\top\sigma)\Big] \tag{5.13}$$

where $\Omega^*(u) = \sup\{u^\top\theta \mid \Omega(\theta)\leq 1\}$ is the dual norm of Ω.

- when Ω is the l_p-norm with $p\in[1,\infty]$, then Ω^* is the l_q-norm, with conjugate realtion $\frac{1}{p}+\frac{1}{q}=1$
- $||\cdot||_1^* = ||\cdot||_\infty$ and $||\cdot||_\infty^* = ||\cdot||_1$ and $||\cdot||_2^* = ||\cdot||_2$.

Thus, computing Rademacher complexities is equivalent to computing expectation of norms. When $\Omega = ||\cdot||_2$, we get:

$$\begin{aligned}\mathcal{R}_n(\mathcal{F}) &= \frac{D}{n}\mathbb{E}[||\Phi^\top\sigma||_2] \\ &\leq \frac{D}{n}\sqrt{\mathbb{E}[||\Phi^\top\sigma||_2^2]} \quad \text{(Jensens' inequality apply on } f(x)=x^2) \\ &= \frac{D}{n}\sqrt{\mathbb{E}[\mathrm{tr}(\Phi^\top\sigma\sigma^\top\Phi)]} \quad \text{(holds for any vector)} \\ &= \frac{D}{n}\sqrt{\mathbb{E}[\mathrm{tr}(\Phi^\top\Phi)]} \quad \text{(using that IID such that } \mathbb{E}[\sigma\sigma^\top]=I) \\ &= \frac{D}{n}\sqrt{\sum_{i=1}^{n}\mathbb{E}[\varphi(X_i)^\top\varphi(X_i)]} = \frac{D}{n}\sqrt{\sum_{i=1}^{n}\mathbb{E}||\varphi(X_i)||_2^2} = \frac{D}{\sqrt{n}}\sqrt{\mathbb{E}||\varphi(X)||_2^2}\end{aligned} \tag{5.14}$$

We thus obtain a *dimension-independent* Rademacher complexity that we can use in the summary below.

Example 5.1. Upper-bound the Rademacher complexity for $\Omega = ||\cdot||_1$.

5.5 Putting Things Together (Linear Predictions)

With all the elements above (section 5.3 and 5.4), we can now propose the following general result (where no convexity of the loss function is assumed).

Proposition 5.3 (Estimation Error)**.** Assume a G-Lipschitz-continuous loss function, linear prediction functions with $\mathcal{F} = \{f_\theta(X) = \theta^\top\varphi(X) \mid ||\theta||_2 \leq D\}$, where $\mathbb{E}||\varphi(X)||_2^2 \leq R^2$. Let $\hat{f} = f_{\hat{\theta}} \in \mathcal{F}$ be the minimizer of the empirical risk, then:

$$\mathbb{E}\big[\mathcal{R}(f_{\hat{\theta}})\big] - \inf_{||\theta||_2\leq D}\mathcal{R}(f_\theta) \leq \frac{2GRD}{\sqrt{n}}$$

It is essential to know that $f_{\hat{\theta}}$ here is a random variable.

Proof. Using Proposition 5.1, equation 5.12 and 5.14, we get the desire result. □

Proposition 5.4 (Approximation Error)**.** If we assume that there exists a minimizer θ_* of $\mathcal{R}(f_\theta)$ over $\mathbb{R}^d$, the approximation error is upper-bounded by

$$\begin{aligned}\inf_{||\theta||_2\leq D}\mathcal{R}(f_\theta) - \mathcal{R}(f_{\theta_*}) &\leq G\inf_{||\theta||_2\leq D}\mathbb{E}[|f_\theta(X) - f_{\theta_*}(X)] \quad \text{(}G\text{-Lipschitz-continuous loss function)} \\ &= G\inf_{||\theta||_2\leq D}\mathbb{E}[|\varphi(X)^\top(\theta-\theta_*)] \\ &\leq G\inf_{||\theta||_2\leq D}||\theta-\theta_*||_2\cdot\mathbb{E}[||\varphi(X)||_2^2] \leq GR\inf_{||\theta||_2\leq D}||\theta-\theta_*||_2\end{aligned}$$

This leads to empirical risk minimization error is uppber-bounded by

$$\mathbb{E}[\mathcal{R}(f_{\hat{\theta}})] - \mathcal{R}(f_{\theta_*}) \leq GR \inf_{||\theta||_2 \leq D} ||\theta - \theta_*||_2 + \frac{2GRD}{\sqrt{n}} = GR(||\theta_*||_2 - D)^+ + \frac{2GRD}{\sqrt{n}} \tag{5.15}$$

We see that for $D = ||\theta_*||_2$, we obtain the bound $\frac{2GR||\theta_*||_2}{\sqrt{n}}$, but this setting requires to know $||\theta_*||_2$ which is not possible in practice.

- if D is too large, the estimation error gets larger, leading to overfitting;
- while if D is too small, the approximation error can quickly kick in (with a value that does not go to zero when n tends to infinity), leading to underfitting.

5.6 From Constrained to Regularized Estimation

In practice, it is preferable to penalize by the norm $\Omega(\theta) = ||\theta||_2$ instead of constraining (the main reasons being that the hyperparameter is easier to find and the optimization is easier).

For simplicity, we only consider the l_2-norm here. We now denote $\hat{\theta}_\lambda$ the minimizer of

$$\hat{\mathcal{R}}(f_\theta) + \frac{\lambda}{2}||\theta||_2^2 \tag{5.16}$$

If the loss is always positive, then

$$\frac{\lambda}{2}||\hat{\theta}_\lambda||_2^2 \leq \hat{\mathcal{R}}(f_{\hat{\theta}_\lambda}) + \frac{\lambda}{2}||\hat{\theta}_\lambda||_2^2 \leq \hat{\mathcal{R}}(f_0)$$

leading to a bound $||\hat{\theta}_\lambda||_2 = \mathcal{O}(1/\sqrt{\lambda})$. Thus, with $D = \mathcal{O}(1/\sqrt{\lambda})$ in the bound above, this lead to a deviation of $\mathcal{O}(1/\sqrt{\lambda n})$, which is not optimal.

We now cite Sridharan, Shalev-Shwartz, and Srebro 2008 without proof an interesting stronger result using the strong convexity of the squared l_2-norm.

Proposition 5.5 (Fast Rates for Regularized Objectives)**.** Assume a G-Lipschitz-continuous **convex** loss function, linear prediction functions with $\mathcal{F} = \{f_\theta(X) = \theta^\top \varphi(X) \mid ||\theta||_2 \leq D\}$, where $\mathbb{E}||\varphi(X)||_2^2 \leq R^2$. Let $\hat{\theta}_\lambda \in \mathbb{R}^d$ be the minimizer of the regularized empirical risk in equation 5.16, then

$$\mathbb{E}[\mathcal{R}(f_{\hat{\theta}_\lambda})] \leq \inf_{\theta \in \mathbb{R}^d} \left\{ \mathcal{R}(f_\theta) + \frac{\lambda}{2}||\theta||_2^2 \right\} + \frac{32G^2R^2}{\lambda n}$$

Note that we obtain a ”fast rate” in $\mathcal{O}(R^2/(\lambda n))$, which has a better dependence in n, but depends on λ, which can be very small in practice. One classical choice of λ if $\lambda \propto GR/(\sqrt{n}||\theta_*||)$, leading to the slow rate

$$\mathbb{E}[\mathcal{R}(f_{\theta_*})] \leq \mathcal{R}(f_{\theta_*}) + \mathcal{O}\left(\frac{GR}{\sqrt{n}}||\theta_*||_2\right)$$

6 Growth Function and VC-Dimension

6.1 Growth Function

Here we will show how the Rademacher complexity can be bounded in terms of the growth function in binary classification problem. To begin with, recall that the empirical Rademacher complexity with respect to sample S with size n is defined as

$$\hat{R}_S(\mathcal{H}) = \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i h(X_i) \right]$$

Definition 6.1 (Growth Function)**.** The growth function $\Pi_{\mathcal{H}} : \mathbb{N} \mapsto \mathbb{N}$ for a hypothesis set $\mathcal{H}$ is defined by

$$\forall\ n \in \mathbb{N}_+,\ \Pi_{\mathcal{H}}(n) = \max \left| \left\{ (h(X_1), \ldots, h(X_n)) \mid h \in \mathcal{H},\ X_1, \ldots, X_n \in \mathcal{X} \right\} \right| \tag{6.1}$$

where $|\cdot|$ compute the cardinality of a set.

Thus, $\Pi_{\mathcal{H}}(n)$ is the maximum number of distinct ways in which n points can be classified using hypotheses in $\mathcal{H}$. This provides another measure of the richness of the hypothesis set $\mathcal{H}$. However, unlike the Rademacher complexity, this measure does not depend on the distribution, it is purely **combinatorial**. To relate the Rademacher complexity to the growth function, we will use Massart's lemma.

Theorem 6.1 (Massart's Lemma)**.** Let $A \subset \mathbb{R}^n$ be a finite set, with $r = \sup_{X \in A} ||X||_2$, then the following holds:

$$\mathbb{E}_\sigma \left[\sup_{X \in \mathcal{A}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i X_i \right] \leq \frac{r\sqrt{2 \log |A|}}{n} \tag{6.2}$$

where σ_i's are independent Rademacher variables taking values in $\{-1, +1\}$ and $X_1, \ldots, X_n$ are the components of vector X.

Proof. For any $t > 0$, using Jensen's inequality, rearranging terms, and bounding the supremum by a sum, we obtain:

$$\begin{aligned}
\exp\left(t \cdot \mathbb{E}_\sigma \left[\sup_{X \in A} \sum_{i=1}^{n} \sigma_i X_i \right] \right) &\leq \mathbb{E}_\sigma \left[\exp\left(t \sup_{X \in A} \sum_{i=1}^{n} \sigma_i X_i \right) \right] \\
&= \mathbb{E}_\sigma \left[\sup_{X \in A} \exp\left(t \sum_{i=1}^{n} \sigma_i X_i \right) \right] \\
&\leq \sum_{X \in A} \mathbb{E}_\sigma \left[\exp\left(t \sum_{i=1}^{n} \sigma_i X_i \right) \right]
\end{aligned}$$

We next use the independence of the σ_i's, then apply the bound in Eq.(C.14), and the definition of r to write:

$$\exp\left(t \cdot \mathbb{E}_\sigma \left[\sup_{X\in A} \sum_{i=1}^n \sigma_i X_i\right]\right) \leq \sum_{X\in A} \prod_{i=1}^n \mathbb{E}[\exp(t\sigma_i X_i)]$$
$$\leq \sum_{X\in A} \prod_{i=1}^n \exp\left(\frac{t^2(2X_i)^2}{8}\right)$$
$$= \sum_{X\in A} \exp\left(\frac{t^2}{2}\sum_{i=1}^n X_i^2\right)$$
$$\leq \sum_{X\in A} \exp\left(\frac{t^2r^2}{2}\right) = |A| \cdot \exp\left(\frac{t^2r^2}{2}\right)$$

The last inequality holds by applying he definition of r, which is

$$r := \sup_{X\in\mathcal{A}} ||X||_2 = \sup_{X\in\mathcal{A}} \sqrt{\sum_{i=1}^n X_i^2}$$

Taking the logarithm on both sides and dividing by t yields:

$$\mathbb{E}_\sigma \left[\sup_{X\in A} \sum_{i=1}^n \sigma_i X_i\right] \leq \frac{\log|A|}{t} + \frac{tr^2}{2} \tag{6.3}$$

Since such inequality holds for every t, we can minimize over t and get $t = \frac{\sqrt{2\log|A|}}{r}$ and get

$$\mathbb{E}_\sigma \left[\sup_{X\in A} \sum_{i=1}^n \sigma_i X_i\right] \leq r\sqrt{2\log|A|}$$

Dividing both sides by n leads to the desired result.

□

Using this result, we can bound the Rademacher complexity $R_n(\mathcal{H})$ in terms of the growth function $\pi_{\mathcal{H}}$.

Corollary 6.2. Let $\mathcal{H}$ be a family of functions taking values in $\{-1, +1\}$. Then the following holds:

$$R_n(\mathcal{H}) \leq \sqrt{\frac{2\log\Pi_{\mathcal{H}}(n)}{n}} \tag{6.4}$$

Proof. For a fixed sample $S_n = (X_1, \dots, X_n) \sim P$, we denote by H_{S_n} the set of vectors of function values $(h(X_1), \dots, h(X_n))^\top$ where h is in $\mathcal{H}$. Singce $h \in \mathcal{H}$ take values in $\{-1, +1\}$, the norm of these vectors is bounded by $\sqrt{n}$. We can then apply Massart's lemma as follows:

$$R_n(\mathcal{H}) = \mathbb{E}_P\left[\mathbb{E}_\sigma\left[\sup_{u\in H_{S_n}} \frac{1}{n}\sum_{i=1}^n \sigma_i u_i\right]\right] \leq \mathbb{E}_P\left[\frac{\sqrt{n}\sqrt{2\log|H_{S_n}|}}{n}\right]$$

By definition, $|H_{S_n}|$ is bounded by the growth function $\Pi_{\mathcal{H}}(n)$, thus,

$$R_n(\mathcal{H}) \leq \mathbb{E}_P\left[\frac{\sqrt{n}\sqrt{2\log\Pi_{\mathcal{H}}(n)}}{n}\right] = \sqrt{\frac{2\log\Pi_{\mathcal{H}}(n)}{n}}$$

which concludes the proof.

□

Combining the generalization bound via Rademacher complexity in Thm. 5.3 with the corollary above yields immediately the following generalization bound in terms of the growth function.

Theorem 6.3 (Generalization Bound via Growth Function)**.** Let $\mathcal{H}$ be a family of functions taking values in $\{-1, +1\}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, we have

$$\mathcal{R}(h) \leq \hat{\mathcal{R}}(h) + 2\sqrt{\frac{2\log \Pi_{\mathcal{H}}(n)}{n}} + \sqrt{\frac{\log(2/\delta)}{2n}} \tag{6.5}$$

$h \in \mathcal{H}$. Again, recall that $\mathcal{R}(h) = \mathbb{E}[h(Z)]$ and $\hat{\mathcal{R}}(h) = \frac{1}{n}\sum_{i=1}^{n} h(Z_i)$.

Growth function bounds can also be derived directly (withougt using Rademacher complexity bounds first). The resulting bound is

$$\mathbb{P}\left(\left|\mathcal{R}(h) - \hat{\mathcal{R}}(h)\right| > \varepsilon\right) \leq 4\Pi_{\mathcal{H}}(2n)\exp\left(-\frac{n\varepsilon}{8}\right) \tag{6.6}$$

The computation of the growth function may not be always convenient since, by definition, it requires computing $\Pi_{\mathcal{H}}(n)$ for all $n \geq 1$. The next section introduces an alternative measure of the complexity of a hypothesis set H that is based instead on a single scalar, which will turn out to be in fact deeply related to the behavior of the growth function.

6.2 VC-dimension

Here, we introduce the notion of VC-dimension (Vapnik-Chervonenkis dimension). The VC-dimension is also a purely combinatorial notion but it is often easier to compute than the growth function (or the Rademacher Complexity). As we shall see, the VC-dimension is a key quantity in learning and is directly related to the growth function.

To define the VC-dimension of a hypothesis class $\mathcal{H}$, we first introduce the concepts of *dichotomy* and that of *shattering*. Given a hypothesis set $\mathcal{H}$, a dichotomy of a set S is one of the possible ways of labeling the points of S using a hypothesis in $\mathcal{H}$. A set S of $n \geq 1$ is said to be shattered by a hypothesis class $\mathcal{H}$ when $\mathcal{H}$ realizes all possible dichotomies of S, that is when $\Pi_{\mathcal{H}}(n) = 2^n$.

Definition 6.2 (VC-dimension)**.** The VC-dimension of a hypothesis class $\mathcal{H}$ is the size of the largest sample set that can be fully shattered by $\mathcal{H}$:

$$\mathrm{VCdim}(H) = \max\{n : \Pi_{\mathcal{H}}(n) = 2^n\} \tag{6.7}$$

Remark 6.1. Note that, by definition, if $\mathrm{VCdim}(\mathcal{H}) = d$, there exists a sample set of size d that can be fully shattered. But, this does not imply that all sets of size d or less are fully shattered, in fact, this is typically not the case.

In general, to compute the VC-dimension, we will typically show a lower bound for its value and then a matching upperbouond. To given a lower bound d for $\mathrm{VCdim}(\mathcal{H})$, it suffices toshow that a set S of cardinality d can be shattered by $\mathcal{H}$. To give an upper bound, we need to prove that no set S of cardinality $d + 1$ can be shattered by $\mathcal{H}$, which is typically more difficult. The followings are some examples of classifers and their VC dimension.

- **Interval Classifier on real line**. Consider a hypothesis class $\mathcal{H} = \{h_{[a,b]} \mid \forall\ a < b\}$ where

$$h_{[a,b]}(X) = \begin{cases} +1, & x \in [a,b] \\ -1, & x \notin [a,b] \end{cases}$$

  It can be shown that $\text{VCdim}(\mathcal{H}) = 2$ in this case. Suppose there is a sample set S with two random variables $(X_1, X_2) = (x_1, x_2)$. Without loss of generality, we suppose $x_1 < x_2$. Then, all four possible dichotomies $(+1, +1)$, $(-1, +1)$, $(+1, -1)$ and $(-1, -1)$ can be realized by some classifer $h_{[a,b]}$. In contrast, by the definition of intervals, no set of three point can be shattered since the case $(+1, -1, +1)$ labeling cannot be realized by any $h_{[a,b]}$. Hence,

$$\text{VCdim}(\text{intervals in } \mathbb{R}) = 2$$

- **Hyperplane Classifier**.

$$\text{VCdim}(\text{hyperpalnes in } \mathbb{R}^d) = d + 1$$

  To begin with, we derive a lower bound by starting with a set of $d + 1$ points in $\mathbb{R}^d$, setting X_0 to be the origin and defining X_i, for $i \in \{1, \ldots, d\}$, as the point whose ith coordinate is 1 and other points are 0, that is,

$$X_{ii} = 1 \quad \text{and} \quad X_{ij} = 0\ \forall j \neq i$$

  for all $d + 1$ points. Let $Y_0, Y_1, \ldots, Y_d \in \{-1, +1\}$ be an arbitrary set of labels for $X_0, X_1, \ldots, X_d$. Let w be the vector whose ith coordinate is Y_i. Then the classifier defined by the hyperplane $\{x \mid w^\top X + Y_0/2 = 0\}$ shatters $X_0, X_1, \ldots, X_d$ since for any $i \in \{0, 1, \ldots, d\}$,

$$\text{sgn}\left(w^\top X_i + \frac{Y_0}{2}\right) = \text{sgn}\left(Y_i + \frac{Y_0}{2}\right) = Y_i \tag{6.8}$$

  To obtain an upper bound, it suffices to show that no set of $d+2$ points can be shattered by halfspaces. Concretely, let S be a set of $d + 2$ points. By Radon's Theorem 6.4, it can be partitioned into two sets X_1 and X_2 such that their convex hulls intersect. Observe that when two sets of points S_1 and S_2 are separaetd by a hyperplane, and each of their convex hulls are also separated by that hyperplane. Thus, S_1 and S_2 cannot be separated by a hyperplane and S is not shattered.

  Combining our lower and upper bounds, we have proven that VC-dimension is $d + 1$ in this case.

- **Axis-ligned Rectangles**.

$$\text{VCdim}(\mathcal{H}) = 4$$

  We first show that the VC-dimension is at least four, by considering four points in a diamond pattern. Then it is clear that all 16 dichotomies can be realized.

- **Convex Polygons**.

- **Sine Functions**.

  The previous examples could suggest that the VC-dimension of $\mathcal{H}$ coincides with the number of free parameters defining $\mathcal{H}$. For example, the number of parameters defining hyperplanes matches their VC-dimension. However, this does not hold in general.

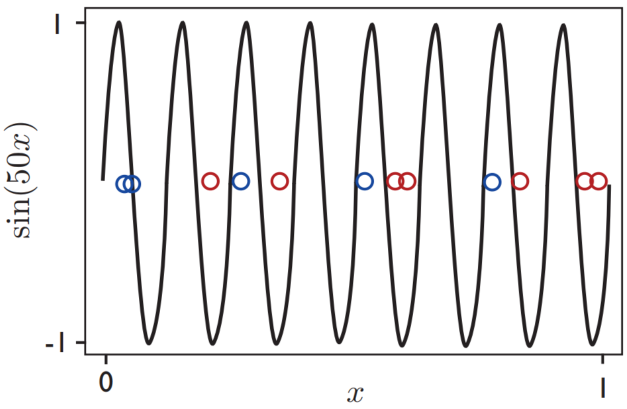


Figure 7: An example of a sine function used for classification

Here is a striking example. Consider the following of sine functions:

$$\mathcal{H} = \{t \mapsto \sin(\omega t) \mid \omega \in \mathbb{R}\}$$

These singe function can be used to classifiy the points on the real line: a point is labeled positively if it is above the curve, negatively otherwise. Altough this family of sine function is defined via a single parameter, ω, it can be shown that VCdim(sine functions) $= +\infty$.

Theorem 6.4 (Radon's theorem)**.** Any set S of $d+2$ points in $\mathbb{R}^d$ can be partitioned into two subsets S_1 and S_2 such that the convex hulls of S_1 and S_2 intersect.

Proof. Let $S = \{X_1, \ldots, X_{d+2}\} \subset \mathbb{R}^d$. The following is a system of $d+1$ linear equations in $\alpha_1, \ldots, \alpha_{d+2}$,

$$\sum_{i=1}^{d+2} \alpha_i X_i = 0 \quad \text{and} \quad \sum_{i=1}^{d+2} \alpha_i = 0$$

This is because the first equality leads to d equations, one for each component of point. The number of unknown, $d+2$, is large than the number of equations, $d+1$, and therefore the system admits a non-zero solution $\beta_1, \ldots, \beta_{d+2}$.

Since $\sum_{i=1}^{d+2} \beta_i = 0$, both $I_1 = \{i \in [1, d+2] \mid \beta_i > 0\}$ and $I_2 = \{i \in [1, d+2] \mid \beta_i < 0\}$ are non-empty sets. Then $S_1 = \{X_i \mid i \in I_1\}$ and $S_2 = \{X_i \mid i \in I_2\}$ form a partition of S. By the last equation above, we have

$$\sum_{i \in I_1} \beta_i = -\sum_{i \in I_2} \beta_i$$

Let $\beta = \sum_{i \in I_1} \beta_i$, then the first part $\sum_{i=1}^{d+2} \alpha_i X_i = 0$ implies that

$$\sum_{i \in I_1} \frac{\beta_i}{\beta} X_i = \sum_{i \in I_2} \frac{-\beta_i}{\beta} X_i$$

with $\sum_{i \in I_1} \beta_i / \beta = 1 = \sum_{i \in I_2} -\beta_i / \beta$, and $\beta_i / \beta \geq 0$ for $i \in I_1$ and $\frac{-\beta_i}{\beta} \geq 0$ for $i \in I_2$. By definition of the convex hulls, this implies that $\sum_{i \in I_1} \frac{\beta_i}{\beta} X_i$ belongs both to the convex hull of S_1 and to that of S_2.

□

6.3 Link Growth Function and VC-dimension

We have shown that the VC-dimension of many other hypothesis sets can be determined or uppder bounded in a similar way. In particular, the VC-dimension of any vector space of dimension $r < \infty$ can be shown to be at most r. The next result known as Sauer's lemma clarifies the connection between the notions of growth function and VC-dimension.

Theorem 6.5 (Sauer's lemma)**.** *Let $\mathcal{H}$ be a hypothesis set with* $\mathrm{VCdim}(\mathcal{H}) = d$*. Then, for all $m \in \mathbb{N}$, the following inequality holds:*

$$\Pi_{\mathcal{H}}(n) \leq \sum_{i=0}^{d} \binom{n}{i} \tag{6.9}$$

Proof. The proof is by induction on $n + d$. The statement clearly holds for $n = 1$ and $d = 0$ or $d = 1$. Now, assume that it holds for $(n - 1, d - 1)$ and $(n - 1, d)$. Fix a sample set $S = \{x_1, \ldots, x_n\}$ with $\Pi_{\mathcal{H}}(n)$ dichotomies and let $G = \mathcal{H}_S$ be the set of concepts $\mathcal{H}$ induces by restriction to S.

Now consider the following families over $S' = \{x_1, \ldots, x_{n-1}\}$. We define $G_1 = G_S$ as the set of concepts $\mathcal{H}$ includes by restriction to S'. Next, ...

□

Corollary 6.6. *Let $\mathcal{H}$ be a hypothesis set with* $\mathrm{VCdim}(\mathcal{H}) = d$*. Then for all $n \geq d$,*

$$\Pi_{\mathcal{H}}(n) \leq \left(\frac{en}{d}\right)^{d} = \mathcal{O}(n^d) \tag{6.10}$$

Proof. The proof begins by using Sauer's lemma. The first inequality multiplies each summand by a factor that is greater than or equal to one since $n \geq d$, while the second inequality adds non-negative summands to the summation.

$$\begin{aligned}
\Pi_{\mathcal{H}}(n) &\leq \sum_{i=0}^{d} \binom{n}{i} \\
&\leq \sum_{i=0}^{d} \binom{n}{i} \left(\frac{n}{d}\right)^{d-i} \\
&\leq \sum_{i=0}^{n} \binom{n}{i} \left(\frac{n}{d}\right)^{d-i} \\
&= \left(\frac{n}{d}\right)^{d} \sum_{i=0}^{d} \binom{n}{i} \left(\frac{d}{n}\right)^{i} \\
&= \left(\frac{n}{d}\right)^{d} \left(1 + \frac{d}{n}\right)^{n} \leq \left(\frac{n}{d}\right)^{d} e^{d}
\end{aligned}$$

After simplifying the expression using the binomial theorem, the final inequality follows using the general identity $(1 + x) \leq e^x$.

□

The explicit relationship just formulated between VC-dimension and the growth function combined with corollary above leads immediately to the following generalization bounds based on the VC-dimension.

Theorem 6.7 (Generalization Bounds via VC-dimension)**.** *Let $\mathcal{H}$ be a family of functions taking values in $\{-1, +1\}$ with VC-dimension d. Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $h \in \mathcal{H}$:*

$$\mathcal{R}(h) \leq \hat{\mathcal{R}}(h) + \sqrt{\frac{2d \log(en/d)}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}} \tag{6.11}$$

Thus, the form of this generalization bound is

$$\mathcal{R}(h) \leq \hat{\mathcal{R}}(h) + \mathcal{O}\left(\sqrt{\frac{\log(n/d)}{(n/d)}}\right) \tag{6.12}$$

which emphasizes the importance of the ratio m/d for generalization. The theorem provides another instance of Occam's razor principle where simplicity is measured in terms of smaller VC-dimension.

VC-dimension bounds can be derived directly without using an intermediate Rademacher complexity bound, as shown in (6.6). Combining Sauer's lemma with (6.6) leads to the following high-probability bound

$$\mathcal{R}(h) \leq \hat{\mathcal{R}}(h) + \sqrt{\frac{8d\log(2em/d) + 8\log(4/\delta)}{n}} \tag{6.13}$$

which has the general form we derive above. The log factor plays only a minor role in these bounds. A finer analysis can be used in fact to eliminate that factor.

6.4 Lower Bounds

See the details in Mohri, Rostamizadeh, and Talwalkar 2018.

7 Covering Number and Chaining

In the case of (binary) classification, we established that only a finite number of elements in the hypothesis class $\mathcal{F}$ really matter, as far as establishing a notion of complexity of $\mathcal{F}$ that can be used to bound uniform deviations in expectation $(\hat{\mathcal{R}}(f) - \mathcal{R}(f))$: only the classifiers yielding different labelings matter. We did so using combinatorial arguments, leading to the notion of complexity given by the growth function, which measures the maximal size of $\mathcal{F}$ when restricted to a given number of points. This quantity, in turn, can be upper-bounded in terms of the VC dimension.

We will now apply the same idea in the setting of regression, where we consider real-valued predictors. We will isolate a few (finitely many) predictors of interest, bound the Rademacher complexity of the set of restrictions to samples in terms of the Rademacher complexity of these representative predictors, and control the error that we commit by only considering a subset of $\mathcal{F}$

Our goal is to find a finite set that explains "most of" the deviation in expectation, up to a certain precision parameter ε. To do so, we will use metric arguments and the notion of covering numbers. This analysis, in fact, will yield improvements also in the setting of binary classification, allowing remove the term $\log(en/d)$ in Eq.(6.11).

7.1 Covering and Packing

We begin by defining the notions of packing and covering a set in a metric space. Recall that a metric space (T, ρ) consists of a non-empty set T, equipped with a mapping $\rho : T \times T \mapsto \mathbb{R}$ that satisfies the following properties:

(a) It is non-negative: $\rho(\theta, \theta')$ for all paris (θ, θ'), with equality if and only if $\theta = \theta'$

(b) It is symmetric: $\rho(\theta, \theta') = \rho(\theta', \theta)$ for all pairs (θ', θ)

(c) The triangle inequality holds: $\rho(\theta, \theta') \leq \rho(\theta, \tilde{\theta}) + \rho(\theta', \tilde{\theta})$

Familiar examples of metric spaces include the real space $\mathbb{R}^d$ wiht the *Euclidean metric*

$$\rho(\theta, \theta') = ||\theta - \theta'||_2 := \sqrt{\sum_{j=1}^{d} (\theta_j - \theta'_j)^2}$$

and the discrete cube $\{0,1\}^d$ with the *rescaled Hamming metric*

$$\rho_H(\theta, \theta') := \frac{1}{d} \sum_{j=1}^{d} \mathbb{1}\{\theta_j \neq \theta'_j\}$$

Also of interest are various metric spaces of functions, among them usual spaces $L^2(\mu, [0,1])$ with its metric

$$||f - g||_2 := \left[\int_0^1 (f(x) - g(x))^2 d\mu(x) \right]^{1/2}$$

as well as the space $C[0,1]$ of all continuous functions on $[0,1]$ equipped with the sup-norm metric

$$||f - g||_\infty = \sup_{x \in [0,1]} |f(x) - g(x)|$$

Given a metric spaces (T, ρ), a natural way in which to measure its size is in terms of number of balls of a fixed radius ε required to cover it, a quantity known as the covering number.

Definition 7.1. A ε-cover of a set T with respect to a metric d is a set $\{\theta_1, \ldots, \theta_n\} \subset T$ such that for each $\theta \in T$, there exists some $i \in \{1, \ldots, n\}$ such that $\rho(\theta, \theta_i) \leq \varepsilon$. The ε-covering number $N(\varepsilon; T, \rho)$ is the cardinality of the smallest ε-cover.

It is easy to see that covering number is decreasing in ε, namely, $N(\varepsilon) \geq N(\varepsilon')$ for all $\varepsilon \leq \varepsilon'$. Typically, the covering number diverges as $\varepsilon \to 0^+$, and of interest to us is this growth rate on a logarithmic scale. More specifically, the quantity

$$\log N(\varepsilon; T, \rho)$$

is known as the *metric entroppy* of the set T with respect to ρ. Here are some examples which show how covering number can be bounded.

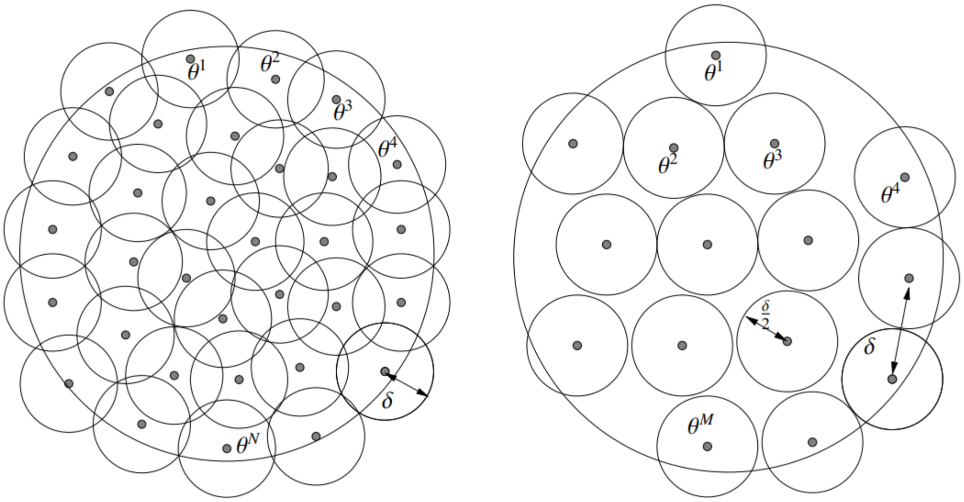


Figure 8: Covering and packing sets

- **Covering numbers of unit cubes**. Consider the interval $[-1, 1]$ in $\mathbb{R}$, equiped with the metric $\rho(\theta, \theta') = |\theta - \theta'|$. Suppose that we divide the interval $[-1, 1]$ into $L := \lfloor 1/\varepsilon \rfloor + 1$ sub intervals, centered at the points $\theta_i = -1 + 2(i-1)\varepsilon$ for $i \in [L] := \{1, 2, \ldots, L\}$, and each of length at most 2ε. By construction, for any point $\theta' \in [0, 1]$, there is some $j \in [L]$ such that $|\theta_j - \theta'| \leq \varepsilon$, which shows that

  $$N(\varepsilon; [-1, 1], |\cdot|) \leq \frac{1}{\varepsilon} + 1$$

  We can easily generalize this analysis for the d-dimensional cube $[-1, 1]^d$, we have

  $$N(\varepsilon; [-1, 1]^d, ||\cdot||_\infty) \leq \left(1 + \frac{1}{\varepsilon}\right)^d$$

- **Covering the binary hypercube**. Consider the binary hypercube $\mathcal{H} = \{0, 1\}^d$ equiped with the rescaled Hamming metrics.

  - First, let us upper bound its ε-covering number. Let $S = \{1, 2, \ldots, \lceil (1-\varepsilon)d \rceil\}$. Consider the set of binary vectors

$$T(\varepsilon) := \{\theta \in H \mid \theta_j = 0,\ \forall\, j \in S\}$$

By construction, for any binary vector $\theta' \in H$, we can find a vector $\theta \in T(\varepsilon)$ such that $\rho_H(\theta, \theta') \leq \varepsilon$. Namely, we can match θ' exactly on all entries $j \in S$, and, in the worst case, disagree on all the remaining $\lfloor \varepsilon d \rfloor$ positions. Since $T(\varepsilon)$ contains $2^{\lceil (1-\varepsilon)d \rceil}$ vectors, we can conclude that

$$\frac{\log N_H(\varepsilon; \mathcal{H}^d)}{\log 2} \leq \lceil (1-\varepsilon)d \rceil$$

– Now let us lower bound its ε-covering number, where $\varepsilon \in (0, 1/2)$. If $\{\theta_1, \dots, \theta_n\}$ is a ε-covering, then the (unrescaled) Hamming balls of radius εd around each θ_l must contain all 2^d vectors in the binary hypercube.

  Let $s = \lfloor \varepsilon d \rfloor$, then for each θ_l, there are exactly $\sum_{j=0}^{s} \binom{d}{j}$ binary vectors lying within distance εd from it, and hence we must have

$$n \cdot \sum_{j=0}^{s} \binom{d}{j} \geq 2^d$$

  where n is the cardinality of delta-covering set. Noq let $X_i \in \{0, 1\}$ be i.i.d. Bernoulli variables with parameter $1/2$. Rearranging the previous inequality, we have

$$\frac{1}{n} \leq \sum_{j=0}^{s} \binom{d}{j} 2^{-d} = \mathbb{P}\left(\sum_{i=1}^{d} X_i \leq \varepsilon d\right) \leq e^{-2d(1/2-\varepsilon)^2}$$

  where the last inequality follows by applying Hoeffding's bound to the sum of d i.i.d. Bernoulli variables. Following some algebra, we obtain the lower bound

$$\log N_H(\varepsilon; \mathcal{H}^d) \geq 2d \left(\frac{1}{2} - \varepsilon\right)^2$$

  valid for $\varepsilon \in (0, 1/2)$. This lower bound is qualitatively correct, but can be tightened by using a better upper bound on the binomial tail probability.

Definition 7.2 (Packing Number)**.** A ε-packing number of a set T with respect to a metric ρ is a set $\{\theta_1, \dots, \theta_m\} \subset T$ such that $\rho(\theta_i, \theta_j) > \varepsilon$ for all distinct $i, j \in \{1, \dots, m\}$. The ε-packing number $M(\varepsilon; T, \rho)$ is the cardinality of the largest ε-packing.

Lemma 7.1. For all $\varepsilon > 0$, the packing and covering numbers are related as follows:

$$M(2\varepsilon; T, \rho) \leq N(\varepsilon; T, \rho) \leq M(\varepsilon; T, \rho) \tag{7.1}$$

7.2 Bound Rademacher Complexity via Covering Number

Recall that in Section 5 where we introduce the Rademacher compelxity, we define a new variable Z over domain $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$, and a function h from hypothesis space $\mathcal{H} = \{h : (Y, X) \mapsto l(Y, f(X)) \mid f \in \mathcal{F}\}$, where $l : \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}$ is some loss function.

Given a sample set $S_n = \{Z_1, \dots, Z_n\} \in \mathcal{Z}^n$, define the following pseudo-norms on the space $\mathcal{H}$: for any

$h \in \mathcal{H}$,

$$\begin{aligned} ||h||_p &:= \left(\frac{1}{n}\sum_{i=1}^{n}|h(X_i)|^p\right)^{1/p}, \quad p \geq 1 \\ ||h||_\infty &:= \max_i |h(X_i)| \end{aligned} \tag{7.2}$$

Note that the reason why we call it pseudo-norm is the space $\mathcal{H}$ is not required to be finite. Now, let $\rho_p(\theta, \theta') := ||\theta - \theta'||_p$ be the pseudo-metric that is induced by the pseudonorms $||\cdot||_p$ on function space $\mathcal{H}$. Then, we can similarily define the covering number $N(\delta; \mathcal{H}, \rho)$ and packing numbers $M(\delta; \mathcal{H}, \rho)$ on pseudo-metric space $(\mathcal{H}, \rho)$.

Lemma 7.2 (Monotonicity)**.** For any $S_n = \{Z_1, \ldots, Z_n\} \in \mathcal{Z}^n$, $1 \leq p \leq q$ and $\delta > 0$, we have

$$N(\delta; \mathcal{H}, \rho_p) \leq N(\delta; \mathcal{H}, \rho_q) \tag{7.3}$$

$$M(\delta; \mathcal{H}, \rho_p) \leq M(\delta; \mathcal{H}, \rho_q) \tag{7.4}$$

Proof. That is because p-norm is decreasing in p when $p \geq 1$. Consider two norms $||\cdot||_p$ and $||\cdot||_q$ of vector x where $1 \leq p \leq q$.

- If $x = 0$, then $||x||_p \geq ||x||_q$ trivially holds;
- If $x > 0$, then let y be a vector such that $y_k = ||x_k||/||x||_q \leq 1$, which means that $y_k^p \geq y_k^q$. Notice that $\sum_k y_k^q = 1$, we have

$$||y||_p \geq 1$$

Hence we have shown that p-norm is decreasing in p, and therefore the covering number with respect to the metric ρ_p induced by p-norm is less than the covering number with respect to metric ρ_q induced by q-norm. □

We next show that the covering numbers of the pseudo-metric space $(\mathcal{F}, \rho_1)$ can be used to bound the empirical Rademacher complexity.

Theorem 7.3 (Bounding Rademacher Complexity via Covering Number)**.** For any fixed sample set $S_n = \{Z_1, \ldots, Z_n\} \in \mathcal{Z}^n$ with size n, let $\sup_{h\in\mathcal{H}} ||h(Z)||_2 \leq c(Z)$, then the empirical Rademacher complexity is bounded by

$$\hat{R}_{S_n}(\mathcal{H}) \leq \inf_{\varepsilon > 0}\left\{\varepsilon + c(Z)\sqrt{\frac{2\log N(\varepsilon; \mathcal{H}, \rho_1)}{n}}\right\} \tag{7.5}$$

recall that ρ_1 is a pseudo-metirc induced by pseudo-norm $||\cdot||_1$, and note that the hypothesis space $\mathcal{H}$ is not required to be finite.

Proof. For a fixed sample $S_n = \{Z_1, \ldots, Z_n\}$ drawn from a unknown joint probability P and $\varepsilon > 0$, we denote by $\mathcal{H}_{S_n}$ the set of vectors of function $H = (h(Z_1), \ldots, h(Z_n))^\top$ where $h \in \mathcal{H}$. Since we know the l_2-norm of function h with respect to Z is bounded by $c(Z)$, i.e. $\sup_{h\in\mathcal{H}} ||h(Z)||_2 \leq c(Z)$, then the norm of these vectors is bounded by $\sqrt{n}c(Z)$, namely

$$\sup_{H\in\mathcal{H}_{S_n}} ||H||_2 = \sup_{h\in\mathcal{H}} \sqrt{\sum_{i=1}^{n} h(Z_i)^2} = \sup_{h\in\mathcal{H}} \sqrt{n}\cdot ||h||_2 \leq \sqrt{n}\cdot c(Z)$$

Now, Let $\mathcal{C} \subset \mathcal{H}$ be a minimal ε-cover of space $(\mathcal{H}; \rho_1)$, and for any $h \in \mathcal{H}$, let $h_0 \in \mathcal{C}$ such that $||h - h_0||_1 \le \varepsilon$. Apply the Massart's lemma, we have

$$\begin{aligned}
\hat{R}_{S_n}(\mathcal{H}) &= \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \sigma_i h(Z_i) \right] \\
&\le \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \sigma_i (h(Z_i) - h_0(Z_i)) \right] + \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \sigma_i h_0(Z_i) \right] \\
&\le \varepsilon + \mathbb{E}_\sigma \left[\sup_{h \in \mathcal{C}} \frac{1}{n} \sum_{i=1}^n \sigma_i h(Z_i) \right] \qquad (7.6) \\
&\le \varepsilon + \sup_{h \in \mathcal{C}} \sqrt{\sum_{i=1}^n h(Z_i)^2} \cdot \frac{\sqrt{2 \log |\mathcal{C}|}}{n} \quad \text{(Massart's lemma in Thm. 6.1)} \\
&\le \varepsilon + c(Z) \sqrt{\frac{2 \log N(\varepsilon; \mathcal{H}, \rho_1)}{n}}
\end{aligned}$$

It is crucial to notice that Massart's lemma only holds on the finite set and here the ε-cover $\mathcal{C}$ meets the requirement. The final result follows by taking the infimum over $\varepsilon > 0$.

□

The bound in Theorem 7.3 establishes a tradeoff with respect to the precision parameter ε, as the decrease of ε woud lead to the increase of covering number $N(\varepsilon; \mathcal{H}, \rho_1)$. In addition, this bound is sample-dependent, namely a random variable, as the right-hand-side depends on $S_n \in \mathcal{Z}^n$

7.3 Chaining

Theorem 7.3 is established by using one fixed level of granularity ($\varepsilon > 0$) at a time, and taking the infimum over $\varepsilon > 0$ to obtain the final bound. An improved version of this result can be established by integrating over different levels of granularity. In this case, we need to work with covering numbers for the pseudo-metric space $(\mathcal{H}, \rho_2)$ where ρ_2 is induced by the pseudo-norm $|| \cdot ||_2$.

Theorem 7.4 (Dudley's Entropy Integral Bound)**.** For any fixed sample set $S_n = (Z_1, \ldots, Z_n) \in \mathcal{Z}^n$ and $\sup_{h \in \mathcal{H}} ||h(Z)||_2 \le c(Z)$, we have

$$\hat{R}_{S_n}(\mathcal{H}) \le \inf_{\varepsilon \in [0, c(Z)/2]} \left\{ 4\varepsilon + \frac{12}{\sqrt{n}} \int_\varepsilon^{c(Z)/2} d\nu \sqrt{\log N(\nu; \mathcal{H}, \rho_2)} \right\} \qquad (7.7)$$

note that the hypothesis space $\mathcal{H}$ is not required to be finite.

Proof. Fix the n-size sample $S_n = \{Z_1, \ldots, Z_n\} \in \mathcal{Z}^n$. For each $j \in \mathbb{N}_+$, let

$$\varepsilon_j := c(Z)/2^j$$

and let $\mathcal{C}_j \subset \mathcal{H}$ be a minimal ε_j-cover of pseudo-metric space $(\mathcal{H}, \rho_2)$. We then have $|\mathcal{C}_j| = N(\varepsilon_j; \mathcal{H}, \rho_2)$. For any $h \in \mathcal{H}$ and $j \in \mathbb{N}_+$, let $h_j \in \mathcal{C}_j$ such that $||h - h_j||_2 \le \varepsilon_j$. The sequence $h_1, h_2, \ldots$ (of elements of cover with decreasing radius) converges towards h. This sequence can be used to define the following telescoping sum, for a given $m \in \mathbb{N}$ to be choose later:

$$h = h - h_m + \sum_{j=1}^{m}(h_j - h_{j-1})$$

with $h_0 := 0$. This telescoping sum can be thought of as a "chain" connecting $h_0 = 0$ to h. This is the reason why the technique we are going to describe is called *chaining*. Upon these, we have

$$\begin{aligned}\hat{R}_{S_n}(\mathcal{H}) &= \mathbb{E}_\sigma\left[\sup_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^{n}\sigma_i h(Z_i)\right] \\ &\leq \mathbb{E}_\sigma\left[\sup_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^{n}\sigma_i (h(Z_i) - h_m(Z_i))\right] + \mathbb{E}_\sigma\left[\sup_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^{n}\sigma_i \sum_{j=1}^{m}(h_j(Z_i) - h_{j-1}(Z_i))\right]\end{aligned}$$

Next, we bound the two summands separately. The first summand is bounded by ε_m as

$$\sum_{i=1}^{n}\sigma_i(h(Z_i) - h_m(Z_i)) \leq \sum_{i=1}^{n}|h(Z_i) - h_m(Z_i)| = n \cdot ||h - h_m||_1 \leq n \cdot ||h - h_m||_2 \leq n \cdot \varepsilon_m$$

Since there are at most $|\mathcal{C}_j| \cdot |\mathcal{C}_{j-1}|$ different ways to create a vector in $\mathbb{R}^n$ of the form

$$\begin{bmatrix} h_j(Z_1) - h_{j-1}(Z_1) \\ \vdots \\ h_j(Z_n) - h_{j-1}(Z_n)\end{bmatrix}$$

with $h_j \in \mathcal{C}_j$ and $h_{j-1} \in \mathcal{C}_{j-1}$, using Massart's lemma in Theorem 6.1 and let $\mathcal{C} = \bigcup_{j=1}^{m}$ be the union of all covers, the second summand can be upper bounded by

$$\begin{aligned}\sum_{j=1}^{m}\mathbb{E}\left[\sup_{h\in\mathcal{H}}\frac{1}{n}\sum_{i=1}^{n}\sum_{i=1}^{n}\sigma_i(h_j(Z_i) - h_{j-1}(Z_i))\right] &= \sum_{j=1}^{m}\mathbb{E}\left[\sup_{h\in\mathcal{C}}\frac{1}{n}\sum_{i=1}^{n}\sum_{i=1}^{n}\sigma_i(h_j(Z_i) - h_{j-1}(Z_i))\right] \\ &\leq \sum_{j=1}^{m}\sup_{h\in\mathcal{C}}\sqrt{\sum_{i=1}^{n}(h_j(Z_i) - h_{j-1}(Z_i))^2} \cdot \frac{\sqrt{2\log|\mathcal{C}_j|\cdot|\mathcal{C}_{j-1}|}}{n} \\ &= \sum_{j=1}^{m}\sup_{h\in\mathcal{C}}||h_j - h_{j-1}||_2 \cdot \sqrt{\frac{2\log|\mathcal{C}_j|\cdot|\mathcal{C}_{j-1}|}{n}}\end{aligned}$$

Here we can see that the $||\cdot||_2$ norm naturally appears in the application of Massart's lemma. With the triangular inequality for the pseudo-norm $||\cdot||_2$, we have (using that $\varepsilon_{k-1} = 2\varepsilon_k$)

$$\begin{aligned}||h_j - h_{j-1}||_2 &\leq ||h_j - h||_2 + ||h - h_{j-1}||_2 \\ &\leq \varepsilon_j + \varepsilon_{j-1} = 3\varepsilon_j = 6(\varepsilon_j - \varepsilon_{j+1})\end{aligned}$$

Also, $|\mathcal{C}_j| = N(\varepsilon_j; \mathcal{H}, \rho_1)$ and $|\mathcal{C}_{j-1}| \leq |\mathcal{C}_j|$. Putting things together, we have

$$\begin{aligned}
\hat{R}_{S_n}(\mathcal{H}) &\leq \varepsilon_m + 12 \sum_{j=1}^{m} (\varepsilon_j - \varepsilon_{j+1}) \sqrt{\frac{\log N(\varepsilon_j; \mathcal{H}, \rho_1)}{n}} \\
&\leq 2\varepsilon_{m+1} + 12 \int_{\varepsilon_{m+1}}^{c(Z)/2} d\nu \sqrt{\log N(\delta; \mathcal{H}, \rho_1)}
\end{aligned}$$

where the last inequality follows as the integral is lower-bound by its lower Riemann sum as the function $\nu \mapsto N(\nu; \mathcal{H}, \rho_1)$ is decreasing. For any $\varepsilon \in [0, c(Z)]/2$, choose m such that $\varepsilon < \varepsilon_{m+1} \leq 2\varepsilon$. The statement of the theorem thus follows by taking the infimum over $\varepsilon \in [0, c(Z)/2]$.

□

8 Optimization for Machine Learning

	Convex	Strongly Convex
Non-smooth	deterministic: $BD/\sqrt{t}$ stochastic: $BD/\sqrt{t}$	deterministic: $B^2/(t\mu)$ stochastic: $B^2/(t\mu)$
Smooth	deterministic: LD^2/t stochastic: $LD^2/\sqrt{t}$ finite sum: n/t	deterministic: $\exp(-t\sqrt{\mu/L})$ stochastic: $L/(t\mu)$ finite sum: $\exp(-t\min\{1/n, \mu/L\})$

Table 1: Above, L is the smoothness constant, μ the strong convexity constant, B the Lipschitz constant and D the distance to optimum at initialization

8.1 Optimization in Machine Learning

In supervised machine learning, we are given n i.i.d. samples (x_i, y_i), $i = 1, \ldots, n$ of a couple of random variables (X, Y) on $\mathcal{X} \times \mathcal{Y}$ and the goal is to find a predictor $f : \mathcal{X} \mapsto \mathbb{R}$ with a small risk

$$\mathcal{R}(f) := \mathbb{E}[l(Y, f(X))]$$

where $l : \mathbb{Y} \times \mathcal{Y} \mapsto \mathbb{R}$ is a loss function. This loss is typlically convex, which is considered as a weak assumption. In the empirical risk minimization (ERM) approach desribed in Section 3, for a parametrization $\{f_\theta\}_{\theta \in \mathbb{R}^d}$ and a regularizer $\Omega : \mathbb{R}^d \mapsto \mathbb{R}$ (e.g. $\Omega(\theta) = ||\theta||_2^2$ or $\Omega(\theta) = ||\theta||_1$), this require to minimize

$$F(\theta) := \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i)) + \Omega(\theta) \tag{8.1}$$

In optimization, the function $F : \mathbb{R}^d \mapsto \mathbb{R}$ is called the objective function.

In general, the minimizer has no closed form. Even when it has one (e.g. linear predictor and square loss), it could be expensive to compute for large problems. We thus resort to iterative algorithms. If the algorithm return $\hat{\theta}$ and let $\theta^* \in \arg\min_\theta \mathcal{R}(f_\theta)$, we can decompose the estimation errpr into (the approximation error due to the selection of hypothesis class Θ is ignored)

$$\mathcal{R}(f_{\hat{\theta}}) - \inf_{\theta \in \mathbb{R}^d} \mathcal{R}(f_\theta) = \underbrace{\{\mathcal{R}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\hat{\theta}})\}}_{\leq \text{estimation error}} + \underbrace{\{\hat{\mathcal{R}}(f_{\hat{\theta}}) - \hat{\mathcal{R}}(f_{\theta^*})\}}_{\leq \text{optimization error}} + \underbrace{\{\hat{\mathcal{R}}(f_{\theta^*}) - \mathcal{R}(f_{\theta^*})\}}_{\leq \text{estimation error}}$$

It is thus sufficient to reach an optimization accuracy of the order of the estimation error (usually of the order $\mathcal{O}(1/\sqrt{n})$ or $\mathcal{O}(1/\sqrt{n})$).

In the following content, we use the notation θ^* for the minimizer of the expected risk and the notation $\theta^\star$ (not $\hat{\theta}$) for the minimizer of the empirical (potentially regularized) risk.

8.2 Gradient Descent on Smooth Problems

Suppose we want to solve, for a function $F : \mathbb{R}^d \mapsto \mathbb{R}$, the optimization problem

$$\min_{\theta \in \mathbb{R}^d} F(\theta)$$

In this section, we do not assume that function F is regularized empirical risk. We further assume that we are given access to certian oracles – the kth-order oracle corresponds to the access to $\theta \mapsto (F(\theta), F'(\theta), \dots, F^{(k)}(\theta))$, that is all partial derivatives up to order k. All algorithms will call these oracles and thus their computational complexity will depend directly on the complexity of this oracle.

We will study the following first-order algorithm: pick $\theta_0 \in \mathbb{R}^d$ and for $t \geq 1$, let

$$\theta_t = \theta_{t-1} - \gamma_t F'(\theta_{t-1}) \tag{8.2}$$

for a well (potentially adaptively) chosen step-size sequence $(\gamma_t)_{t\geq 1}$. There are many ways to choose the step-size γ_t, either constant, either decaying, either through a line search. In practice, using some form of line search is strongly advantageous and is implemented in most applicaiton. In this section, to simplify the algorithms and proofs, we will focus on constant or iteration-dependent step-size.

Note that, for machine learning problem where the empirical risk is minimized, computing the gradient $F'(\theta_{t-1})$ requires computing all gradients of $\theta \mapsto l(y_i, f_\theta(x_i))$ for $i = 1, \dots, n$ and averaging them. In this context, gradient descent on the empirical risk, is often called a "batch" technique (compared with stochastic technique), because all the data points are accessed at every iteration.

8.2.1 Analysis of GD for ordinary least squares

We first start with the simplest example, namely the quadratic convex functions (which is strongly convex), which is just the loss function in ordinary least squares. Let $\Phi \in \mathbb{R}^{n\times d}$ be the design matrix, and $y \in \mathbb{R}^n$ the vector of responses. Least-squares estimation amoutns to finding a minimizer $\theta^\star$ of

$$F(\theta) = \frac{1}{2n}||\Phi\theta - y||_2^2 = \frac{1}{2n}(y - \Phi\theta)^\top (y - \Phi\theta)$$

The gradient of F is $F'(\theta) = \frac{1}{n}\Phi^\top(\Phi\theta - y) = \frac{1}{n}\Phi^\top\Phi\theta - \frac{1}{n}\Phi^\top y$. Thus, denoting $H = \frac{1}{n}\Phi^\top\Phi \in \mathbb{R}^{d\times d}$ the Hessian matrix (with respect to θ), the minimizers $\theta^\star$ are characterized by

$$F'(\theta^\star) = 0 \quad \Rightarrow \quad H\theta^\star = \frac{1}{n}\Phi^\top y \tag{8.3}$$

Since $\frac{1}{n}\Phi^\top y \in \mathbb{R}^d$ is in the range space of H, there is always a minimizer, but unless H is invertible, the minimizer is not unique. But all minimizers $\theta^\star$ have the same function value $F(\theta^\star)$, and we have, from a simple Taylor expansion

$$\begin{aligned} F(\theta) - F(\theta^\star) &= F'(\theta^\star)^\top(\theta - \theta^\star) + \frac{1}{2}(\theta - \theta^\star)^\top H(\theta - \theta^\star) \\ &= \frac{1}{2}(\theta - \theta^\star)^\top H(\theta - \theta^\star) \end{aligned}$$

Suppose $M := \lambda_{\max}(H)$ and $m := \lambda_{\min}(H)$ be the largest and smallest eigenvalues of the Hessian matrix H. We denote by $\kappa = M/m \geq 1$ the condition number.

Closed-form expression. Gradient descent iterates with fixed step-size $\gamma_t = \gamma$ can be computed in closed form:

$$\begin{aligned} \theta_t = \theta_{t-1} - \gamma F'(\theta_{t-1}) &= \theta_{t-1} - \gamma\left[\frac{1}{n}\Phi^\top(\Phi\theta_{t-1} - y)\right] \\ &= \theta_{t-1} - \gamma H(\theta_{t-1} - \theta^\star) \end{aligned}$$

leading to

$$\theta_t - \theta^\star = \theta_{t-1} - \theta^\star - \gamma H(\theta_{t-1} - \theta^*) = (I - \gamma H)(\theta_{t-1} - \theta^\star)$$

that is, we have linear recursion, and we can unroll the recursion and write

$$\theta_t - \theta^\star = (I - \gamma H)^t(\theta_0 - \theta^\star)$$

We can now look at various measures of performace:

$$||\theta_t - \theta^\star||_2^2 = (\theta_0 - \theta^\star)^\top (I - \gamma H)^{2t}(\theta_0 - \theta^\star)$$
$$F(\theta_t) - F(\theta^\star) = \frac{1}{2}(\theta_0 - \theta^\star)^\top (I - \gamma H)^{2t} H(\theta_0 - \theta^\star)$$

Note that the second equality holds by applying $H\theta^\star = \frac{1}{n}\Phi^\top y$.

8.2.2 Analysis of GD for strongly and smooth functions

The analysis of optimization algorithms requires assumptions on the objective functions, like the ones introduced in this section. From these assumptions, additional properties are derived (typically inequalities), and then most convergence proofs look for a ”Lyapunov function” that goes down along the iterations. More precisely, if $V : \mathbb{R}^d \mapsto \mathbb{R}_+$ is such that $V(\theta_t) \leq (1-\alpha)V(\theta_{t-1})$, then $V(\theta_t) \leq (1-\alpha)^t V(\theta_0)$ and we obtain linear convergence rate. The art is then to find the appropriate Lynapunov function.

We first consider an assumption allowing exponential convergence rates.

Definition 8.1 (Convex function)**.** A differentiable function $F : \mathbb{R}^d \mapsto \mathbb{R}$ is said to be convex if and only if

$$F(\eta) \geq F(\theta) + F'(\theta)^\top(\eta - \theta), \quad \forall\ \eta, \theta \in \mathbb{R}^d \tag{8.4}$$

this conclusion holds even for $\eta = \theta^\star$.

Definition 8.2 (Strong convexity)**.** A differentiable function F is said μ-strongly convex, with $m > 0$, if and only if

$$F(\eta) \geq F(\theta) + F'(\theta)^\top(\eta - \theta) + \frac{\mu}{2}||\eta - \theta||_2^2 \tag{8.5}$$

for all $\eta, \theta \in \mathbb{R}^d$. For twice differentiable functions, this is equivalent to $F'' \succeq mI$.

The function F is strongly-convex if and only if the function F is strictly above its tangent, and the difference is at least quadratic in the distance to the point where the two coincide. This notably allows to define quadratic lower bounds on F.

Lemma 8.1 (Lojasiewics inequality)**.** If F is differentiable and m-strongly convex with unique minimizer $\theta^\star$, then we have:

$$||F'(\theta)||_2^2 \geq 2\mu(F(\theta) - F(\theta^\star))$$

Proof. The right-hand side of Eq.(8.5) is strongly convex in η and minimized with $\eta = \theta - \frac{1}{\mu}F'(\theta)$. Plugging this value into the bound and letting $\eta = \theta^\star$, we get

$$F(\theta^\star) \geq F(\theta) - \frac{1}{\mu}||F'(\theta)||_2^2 + \frac{1}{2\mu}||F'(\theta)||_2^2 = F(\theta) - \frac{1}{2\mu}||F'(\theta)||_2^2$$

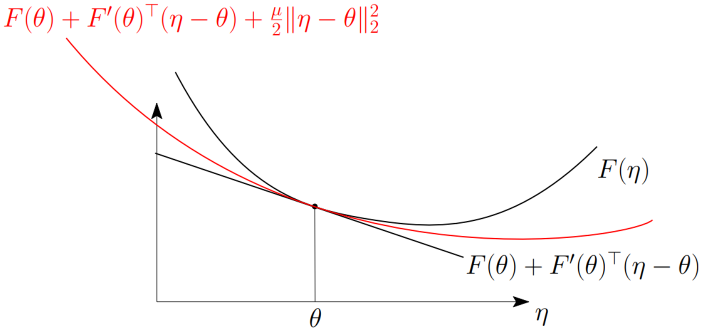

$F(\theta) + F'(\theta)^\top(\eta-\theta) + \frac{\mu}{2}\|\eta-\theta\|_2^2$
$F(\eta)$
$F(\theta) + F'(\theta)^\top(\eta-\theta)$
θ
η

Figure 9: Strong convexity

The conclusion follows by rearranging.

□

In order to obtain exponential convergence rates, strong-convexity is typically associated with smoothness, which we now define.

Definition 8.3 (Smoothness)**.** A differentiable function F is said L-smooth if and only if

$$|F(\eta) - F(\theta) - F'(\theta)^\top(\eta-\theta)| \leq \frac{L}{2}||\eta-\theta||_2^2 \quad \forall\ \theta,\eta\in\mathbb{R}^d \tag{8.6}$$

which is equivalent to F having a L-Lipschitz-continuous gradient,

$$||F'(\theta) - F'(\eta)||_2^2 \leq L^2||\theta-\eta||_2^2$$

and for twice differentiable functions, this is equivalent to $-LI \preceq F''(\theta) \preceq LI$.

Note that when F is convex and L-smooth, we have a quadratic upper-bound which is tight at any given point (strong convexity implies the corresponding lower bound), i.e.,

$$F(\eta) \leq F(\theta) + F'(\theta) + F'(\theta)^\top(\eta-\theta) + \frac{L}{2}||\eta-\theta||_2^2$$

For machine learning problems with linear predictions and smooth losses (squared or logistic), we have smooth problems. If we use a squared l_2-regularizer $\frac{\mu}{2}||\cdot||_2^2$, we get a μ-strongly convex problem. Note that when using regularization, the value of μ decays with n, typically between $1/n$ and $1/\sqrt{n}$, leading to condition numbers κ bewtween $\sqrt{n}$ and n.

In the next theorem, we show that gradient descent converges exponentially for such smooth and strongly-convex problems.

Theorem 8.2 (Convergence of GD for smooth strongly-convex functions)**.** Assume that F is L-smooth and μ-strongly convex. Choosing step-size $\gamma_t = 1/L$, the iterates $(\theta_t)_{t\geq 0}$ of Gradient Descent on F satisfy

$$F(\theta_t) - F(\theta^\star) \leq \left(1 - \frac{\mu}{L}\right)^t \cdot (F(\theta_0) - F(\theta^\star)) \leq e^{-t\mu/L}\cdot(F(\theta_0) - F(\theta^\star))$$

Proof. By the smoothness inequality in Eq.(8.6) applied to θ_{t-1} and $\theta_{t-1} - F'(\theta_{t-1})/L$, we have the following

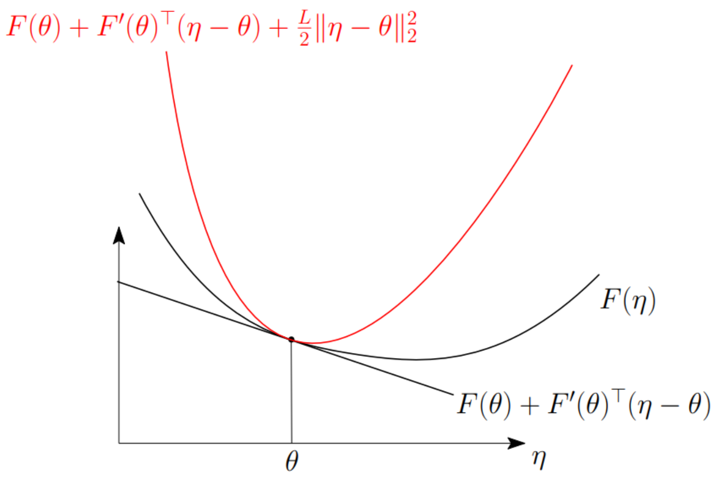

$F(\theta) + F'(\theta)^\top(\eta - \theta) + \frac{L}{2}\|\eta - \theta\|_2^2$
$F(\eta)$
$F(\theta) + F'(\theta)^\top(\eta - \theta)$
θ
η

Figure 10: L-smoothness

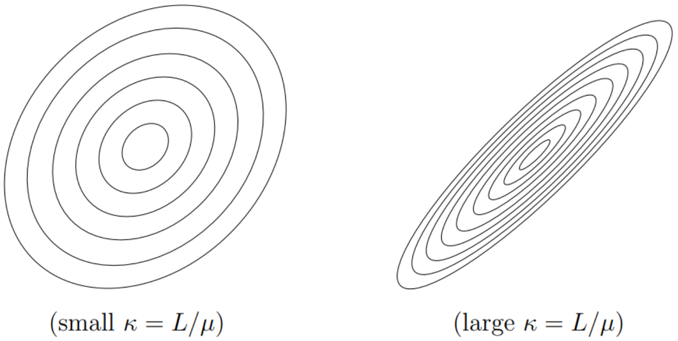


Figure 11: When a function is both smooth and strongly convex, we denote by $\kappa = L/\mu \geq 1$ its condition number, and the condition number impacts the shapes of the level sets

descent property, with $\gamma_t = 1/L$,

$$\begin{aligned} F(\theta_t) = F(\theta_t - F'(\theta_{t-1})/L) &\leq F(\theta_{t-1}) + F'(\theta_{t-1})^\top(-F'(\theta_{t-1})/L) + \frac{L}{2}|| - F'(\theta_{t-1})/L||_2^2 \\ &= F(\theta_{t-1}) - \frac{1}{2L}||F'(\theta_{t-1})||_2^2 \end{aligned} \tag{8.7}$$

Adding $-F(\theta^\star)$ on both sides, we get

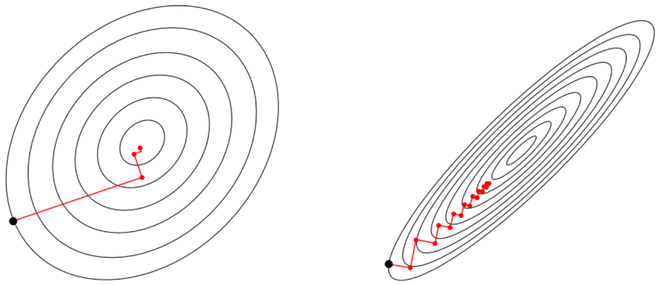
$$F(\theta_t) - F(\theta^\star) \leq (F(\theta_{t-1}) - F(\theta^\star)) - \frac{1}{2L}||F'(\theta_{t-1})||_2^2$$

Using Lojasiewicz inequality (Lemma 8.1), it follows

$$F(\theta_t) - F(\theta^\star) \leq (1 - \mu/L) \cdot (F(\theta_{t-1}) - F(\theta^\star)) \leq e^{-\mu/L} \cdot (F(\theta_{t-1}) - F(\theta^\star))$$

Recursively applying this inequality leads to the desired result.

□



(small $\kappa = L/\mu$) (large $\kappa = L/\mu$)

Figure 12: The performance of gradient descent will depend on this condition number (see the steepest descent, i.e., gradient descent with exact line search): with small condition number (left), we get fast convergence, while for a large condition number (right), we get oscillations

We can make the following observations:

- As mentioned before, we necessarily have $\mu \leq L$; the ratio $\kappa := L/\mu$ is called the condition number
- If we only assume that the function is smooth and convex (not strongly convex), then Gradient Descent with constant step-size $\gamma = 1/L$ also converges when a minimizer exists, but at a slower rate $\mathcal{O}(1/t)$. More details in next section.
- Choosing the step-size only requires an upper bound L on the smoothness constant (in case it is over-estimated, the convergence rate only degrades slightly)

8.2.3 Analysis of GD for convex and smooth functions

In order to obtain the $1/t$ (linear) convergence rate without strong-convexity, we will need an extra property of convex smooth functions, sometimes called ”co-coercivity”. This is an instance of inequalities that we need to use to circumvent the lack of closed form for iterations.

Proposition 8.1 (co-coercivity)**.** If F is a convex L-smooth function on $\mathbb{R}^d$, then for all $\theta, \eta \in \mathbb{R}^d$, we have

$$\frac{1}{L}||F'(\theta) - F'(\eta)||_2^2 \leq [F'(\theta) - F'(\eta)]^\top(\theta - \eta)$$

or equivalently, $F(\theta) \geq F(\eta) + F'(\eta)^\top(\theta - \eta) + \frac{1}{2L}||F'(\theta) - F'(\eta)||_2^2$.

Proof. Define $H(\theta) = F(\theta) - F'(\eta)^\top\theta$. The function $H : \mathbb{R}^d \mapsto \mathbb{R}$ is convex in θ with global minimum at η, and is also L-smooth. Now, we can apply the property of L-smoothness in Eq.(8.6) and get

$$\begin{aligned} H(\eta) \leq H(\theta - H'(\theta)/L) &\leq H(\theta) + H'(\theta)^\top(-H'(\theta)/L) + \frac{L}{2}|| - H'(\theta)/L||_2^2 \\ &= H(\theta) - \frac{1}{2L}||H'(\theta)||_2^2 \end{aligned}$$

This leads to

$$F(\eta) - F'(\eta)^\top\eta \leq F(\theta) - F'(\eta)^\top\theta - \frac{1}{2L}||F'(\theta) - F'(\eta)||_2^2$$

Rearranging the terms leads to the desired result.

□

We can now state the following convergence result for gradient descent with potentially no strong-convexity.

Theorem 8.3 (Convergence of GD for smooth convex functions)**.** Assume that F is L-smooth and convex, with a global minimizer $\theta^\star$. Choosing step-size $\gamma_t = 1/L$, the iterates $(\theta_t)_{t\geq 0}$ of Gradient Descent on F satisfy

$$F(\theta_t) - F(\theta^\star) \leq \frac{L}{2t}||\theta_0 - \theta^\star||_2^2$$

Proof. The Lyapunov function that we will choose is

$$V_t(\theta_t) = t(F(\theta_t) - F(\theta^\star)) + \frac{L}{2}||\theta_t - \theta^\star||_2^2 \tag{8.8}$$

and our goal is to show that it decays along iterations. We can split the difference in Lyapunov functions in three terms

$$V_t(\theta_t) - V_{t-1}(\theta_{t-1}) = \underbrace{tF(\theta_t) - tF(\theta_{t-1})}_{\text{part I}} + \underbrace{F(\theta_{t-1}) - F(\theta^\star)}_{\text{part II}} + \underbrace{\frac{L}{2}||\theta_t - \theta^\star||_2^2 - \frac{L}{2}||\theta_{t-1} - \theta^\star||_2^2}_{\text{part III}}$$

We bound these three parts separately:

- From Eq.(8.7), we have

$$F(\theta_t) - F(\theta_{t-1}) \leq -\frac{1}{2L}||F'(\theta_{t-1})||_2^2$$

- For a convex function, we have

$$F(\theta^\star) \geq F(\theta_{t-1}) + F'(\theta_{t-1})^\top(\theta^\star - \theta_{t-1}) \quad \Rightarrow \quad F(\theta_{t-1}) - F(\theta^\star) \leq F'(\theta_{t-1})^\top(\theta_{t-1} - \theta^\star)$$

- Expanding the difference of square, we have

$$\begin{aligned}||\theta_t - \theta^\star||_2^2 - ||\theta_{t-1} - \theta^\star||_2^2 &= ||\theta_{t-1} - \gamma_t - \theta^\star||_2^2 - -||\theta_{t-1} - \theta^\star||_2^2 \\ &= -2\gamma_t F'(\theta_{t-1})^\top(\theta_{t-1} - \theta^\star) + \gamma_t^2||F'(\theta_{t-1})||_2^2\end{aligned}$$

Hence, with step-size $\gamma_t = 1/L$, we have

$$\begin{aligned}V_t(\theta_t) - V_{t-1}(\theta_{t-1}) &\leq -\frac{t}{2L}||F'(\theta_{t-1})||_2^2 + F'(\theta_{t-1})^\top(\theta_{t-1} - \theta^\star) - F'(\theta_{t-1})^\top(\theta_{t-1} - \theta^\star) + \frac{1}{2L}||F'(\theta_{t-1})||_2^2 \\ &= \frac{1-t}{2L}||F'(\theta_{t-1})||_2^2 \leq 0\end{aligned}$$

which leads to

$$t(F(\theta_t) - F(\theta^\star)) \leq V_t(\theta_t) \leq V_0(\theta_0) = \frac{L}{2}||\theta_0 - \theta^\star||_2^2$$

and thus $F(\theta_t) - F(\theta^\star) \leq \frac{L}{2t}||\theta_0 - \theta^\star||_2^2$.

□

The proof above is on purpose mysterious: the choice of Lyapunov function seems arbitrary at first, but all inequalities lead to nice cancellations. These proofs are sometimes hard to design. See Bach 2021 for more interesting details.

8.2.4 Beyond Gradient Descent

While gradient descent is the simplest algorithm with a simple analysis, there are multiple extensions we will here briefly mention (more details see Yurii Nesterov et al. 2018)

- **Nesterov acceleration**. For convex functions, a simple modification of gradient descent allows to obtain better convergence rates. The algorithm is as follows:

  $$\begin{aligned} \theta_t &= \eta_{t-1} - \frac{1}{L} F'(\eta_{t-1}) \\ \eta_t &= \theta_t + \frac{t-1}{t+2}(\theta_t - \theta_{t-1}) \end{aligned}$$

  This simple modification leads to the following convergence rate

  $$F(\theta_t) - F(\theta^\star) \leq \frac{2L||\theta_0 - \theta^\star||_2^2}{(t+1)^2}$$

  For strongly convex functions, the algorithm has a similar form as for convex functions, but with all coefficients independent from t:

  $$\begin{aligned} \theta_t &= \eta_{t-1} - \frac{1}{L} F'(\eta_{t-1}) \\ \eta_t &= \theta_t + \frac{1-\sqrt{\mu/L}}{1+\sqrt{\mu/L}}(\theta_t - \theta_{t-1}) \end{aligned}$$

  and the convergence rate is

  $$F(\theta_t) - F(\theta^*) \leq L(1-\sqrt{\mu/L})^t ||\theta_0 - \theta^\star||_2^2$$

- **Newton method**. Given θ_{t-1}, the Newton method minimizes the second-order Tarylor expansion around θ_{t-1}:

  $$F(\theta_t) \approx F(\theta_{t-1}) + F'(\theta_{t-1})^\top(\theta - \theta_{t-1}) + \frac{1}{2}(\theta - \theta_{t-1})^\top F''(\theta_{t-1})^\top(\theta - \theta_{t-1})$$

  which leads to the descent algorithm

  $$\theta_t = \theta_{t-1} - F''(\theta_{t-1})^{-1} F'(\theta_{t-1}) \tag{8.9}$$

  This is an expensive iteration, as the running-time compelxity is $\mathcal{O}(d^3)$ in general to solve the linear system (matrix inverse). It leads to local quadratic rate convergence. See S. Boyd, S. P. Boyd, and Vandenberghe 2004 for more details, and for condition for global convergence.

  Note that for machine learning problems, quadratic convergence may be an overkill compared to the computational complexity of each iteration, since cost functions are averages of n terms and naturally have some uncertainty of order $\mathcal{O}(1/\sqrt{n})$.

- **Proximal gradient descent**. Many optimization problem are said ”composite”, that is, the objective function F is the sum of a smooth function G and a non-smooth function H (such as norm). It turns out that a simple modification of gradient descent allows to benefit from the fast convergence rates of smooth optimization.

For this, we need to first see gradient descent as a proximal method. Indeed, one may see the iteration $\theta_t = \theta_{t-1} - \frac{1}{L} G'(\theta_{t-1})$ as

$$\theta_t = \underset{\theta \in \mathbb{R}^d}{\arg\min} \; G(\theta_{t-1}) + G'(\theta_{t-1})^\top (\theta - \theta_{t-1}) + \frac{L}{2} ||\theta - \theta_{t-1}||_2^2$$

where, for a L-smooth function G, the objective function above is an upper-bound of $G(\theta)$, which is tight at θ_{t-1}. While this reformulation does not bring much for gradient descent, we can extend this to the composite problem, and consider the iteration

$$\theta_t = \underset{\theta \in \mathbb{R}^d}{\arg\min} \; G(\theta_{t-1}) + G'(\theta_{t-1})^\top (\theta - \theta_{t-1}) + \frac{L}{2} ||\theta - \theta_{t-1}||_2^2 + H(\theta)$$

where H is left as what it is. The crux is to be able to compute the step above, that is minimize with respect to θ functions of the form $\frac{L}{2} ||\theta - \theta_{t-1}||_2^2 + H(\theta)$. When H is the indicator function of a convex set (which is equal to 0 inside the set, and $+\infty$ otherwise), we get **projected gradient descent**. When H is the l_1-norm, that is $H = \lambda || \cdot ||_1$, this can be shown to be soft-thresholding step, as for coordinate $\theta_i = \eta_i / |\eta_i| (|\eta_i| - \lambda / L)^+$.

It turns out that the convergence rates for G + H are the same as smooth optimization, with potential acceleration (Yu Nesterov 2013).

8.3 Gradient Methods on Non-smooth Problems

We now relax our assumptions and only require Lipschitz continuity (instead of L-smo) in addition to convexity. The rates will be slower, but the extension to stochastic gradients descent is easier.

Definition 8.4 (Lipschitz-continuous function)**.** A function $F : \mathbb{R}^d \mapsto \mathbb{R}$ is said B-Lipschitz-continuous if and only if

$$|F(\eta) - F(\theta)| \leq B ||\eta - \theta||_2, \quad \forall \; \theta, \eta \in \mathbb{R}^d$$

If F is differentiable, this is equivalent to the assumption $||F'(\theta)||_2 \leq B, \; \forall \theta \in \mathbb{R}^d$.

Without additional assumptions, this setting is usually refered to as non-smooth optimization. Now we can apply non-smooth optimization to objective functions which are not differentiable (such as the hinge loss). For convex Lipschitz-continuous objectives, the function is differentiable almost everywhere. In points where it is not, then one can define the set of slopes of lower-bounding tangents as the *subdifferential*, and any element of it as a *subgradient*. The Gradient Descent iteration is then meant as using any subgradient instead of $F'(\theta_{t-1})$, formally,

$$\theta_t = \theta_{t-1} - \gamma_t G_t, \quad G_t \in \partial F(\theta_{t-1})$$

This method is then referred to as the Subgradient Method, and it is not a descent method anymore as the function values may go up once in a while.

We can now prove convergence rate of the Subgradient Method, with a decaying step-size, and a slower rate compared with smooth functions Gradient Descent.

Theorem 8.4 (Convergence of the subgradient method)**.** Assume that F is convex, B-Lipschitz-continuous, and admits a minimizer $\theta^\star$ that satisfies $||\theta^\star - \theta_0||_2 \leq D$. By choosing $\gamma_t = \frac{D}{B\sqrt{t}}$ then the iterates $(\theta_t)_{t \geq 0}$ of Subgradient Method on F satisfy

$$\min_{0 \leq s \leq t-1} F(\theta_s) - F(\theta^\star) \leq DB \frac{2 + \log t}{2\sqrt{t}}$$

Proof. We look at how θ_t approaches $\theta^\star$, that is, we try to use $||\theta_t - \theta^\star||_2^2$ as a Lyapunov function. We have:

$$\begin{aligned} ||\theta_t - \theta^\star||_2^2 &= ||\theta_{t-1} - \gamma_t F'(\theta_{t-1}) - \theta^\star||_2^2 \\ &= ||\theta_{t-1} - \theta^\star||_2^2 - 2\gamma_t F'(\theta_{t-1})^\top (\theta_{t-1} - \theta^\star) + \gamma_t^2 ||F'(\theta_{t-1]})||_2^2 \end{aligned}$$

Combining this with the convexity inequality $F(\theta_{t-1}) - F(\theta^\star) \leq F'(\theta_{t-1})^\top(\theta_{t-1} - \theta^\star)$ from Eq.(8.4), we have (also using the boundedness of gradients/Lipschiz-continuous)

$$||\theta_t - \theta^\star||_2^2 \leq ||\theta_{t-1} - \theta^\star||_2^2 - 2\gamma_t[F(\theta_{t-1}) - F(\theta^\star)] + \gamma_t^2 B^2$$

and thus, by isolating the distance to optimum in function values:

$$\gamma_t(F(\theta_{t-1}) - F(\theta^\star)) \leq \frac{1}{2}\left(||\theta_{t-1} - \theta^\star||_2^2 - ||\theta_t - \theta^\star||_2^2\right) + \frac{1}{2}\gamma_t^2 B^2 \tag{8.10}$$

It is sufficient to sum these inequalities up to t and drop the term $-||\theta_{t+1} - \theta^\star||_2^2$ to get, for any $\theta^\star \in \mathbb{R}^d$,

$$\frac{1}{\sum_{s=1}^t \gamma_s} \sum_{s=1}^t \gamma_s (F(\theta_{s-1}) - F(\theta^\star)) \leq \frac{||\theta_0 - \theta^\star||_2^2}{2\sum_{s=1}^t \gamma_s} + B^2 \frac{\sum_{s=1}^t \gamma_s^2}{2\sum_{s=1}^t \gamma_s}$$

The left-hand side is trivially larger than $\min_{0\leq s\leq t-1}(F(\theta_s) - F(\theta^\star))$, and than $F(\theta_t) - F(\theta^\star)$ where $\bar{\theta}_t = (\sum_{s=1}^t \gamma_s \theta_{s-1})/(\sum_{s=1}^t \gamma_s)$ by Jensen's inequality.

The upper bound goes to zero if $\sum_{s=1}^t \gamma_s \to \infty$ and $\gamma_t \to 0$. Let us choose $\gamma_s = \tau/\sqrt{s}$ for some $\tau > 0$. By using the series-integral comparisons below,

$$\sum_{s=1}^t \frac{1}{\sqrt{s}} \geq \sum_{s=1}^t \frac{1}{\sqrt{t}} = \sqrt{t} \quad \text{and} \quad \sum_{s=1}^t \frac{1}{s} \leq 1 + \sum_{s=2}^t \frac{1}{s} \leq 1 + \int_1^t \frac{ds}{s} = 1 + \log t$$

we get the bound

$$\min_{0\leq s\leq t-1}(F(\theta_s) - F(\theta^\star)) \leq \frac{1}{2\tau\sqrt{t}}\left(D^2 + \tau^2 B^2(1 + \log t)\right)$$

Choosing $\tau = D/B$ leads to the desired results (which is suggested by optimizing the previous bound when $\log t = 0$).

□

The proof scheme above is very flexible and can be extended in the following directions:

- The algorithm applies to **constrained minimization** over a convex set, by inserting a proection step at each iteration (the proof, which is using the contractivity of orthogonal projections, is essentially the same)
- The algorithm applies to **non-differentiable** convex and Lipschitz objective functions using subgradients (any vector satisfying Eq.(8.4 in place of $F'(\theta_t)$)
- The algorithm can be applied to **non-Euclidean geometries**, where we consider bounds on the iterates or the gradient with different quantities. This can be done using ”mirror descent” framework, and for instance can be applied to obtain multiplicative updates
- Often the uniformly averaged iterate, $\frac{1}{t}\sum_{s=0}^{t-1}\theta_s$ is used. Convergence rates without $\log t$ factor can be obtained using Abel summation formula

- Stochastic gradients method can be used, as presented below (one interpretation is that the subgradient method is so slow that it is robust to noisy gradients)

More details see Bach 2021.

8.4 Stochastic Gradient Descent

9 Kernel Methods

In this section, we study empirical risk minimization for linear models, that is, prediction functions $f_\theta : \mathcal{X} \mapsto \mathbb{R}$ which are linear in parameters θ, that is, of the form $f_\theta = \langle \theta, \varphi(x) \rangle_{\mathcal{H}}$ and $\mathcal{H}$ is a Hilbert space and $\theta \in \mathcal{H}$.

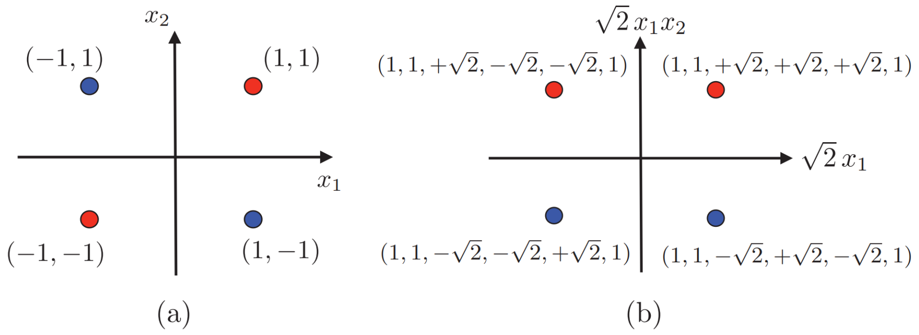
The key difference with least-squares estimation is that, (1) we are not restricted to the square loss, and (2) we explicitly allow infinite-dimensional models, thus extending the dimenison-free bounds from linear least-squares regression (see Chapter 3 in Bach 2021)

Why kernel methods. The study of infinite-dimensional linear models is important for several reasons:

- Understanding linear models in finite but very lage input dimension dimensions requries tools from infinite-dimensional analysis
- Kernel methods lead to simple and stable algorithms, with theoretical guarantess, and adaptivity to smoothness of the target function (as oppsed to local averaging techniques). They can be applied in high dimensions, with good practical performance (not state of arts techinique for CV and NLP compared to NN)
- They can be easily applied when input observations are not vectors
- They are useful to understand other models such as neural networks

9.1 Motivating Example to Kernel Function

Before we go deep into the area of kenrel methods, let's see some examples in classification.



x_2
$(-1,1)$
$(1,1)$
x_1
$(-1,-1)$
$(1,-1)$
(a)
$\sqrt{2}\,x_1x_2$
$(1,1,+\sqrt{2},-\sqrt{2},-\sqrt{2},1)$
$(1,1,+\sqrt{2},+\sqrt{2},+\sqrt{2},1)$
$\sqrt{2}\,x_1$
$(1,1,-\sqrt{2},-\sqrt{2},+\sqrt{2},1)$
$(1,1,-\sqrt{2},+\sqrt{2},-\sqrt{2},1)$
(b)

Figure 13: XOR classification problem

Example 9.1 (XOR Classification)**.** Given two dimensional input features $X = (X_1, X_2)^\top$, we have label $Y = +1$ if and only if $X_1 = X_2$ and $Y = -1$ if and only if $X_1 \neq X_2$. We use red node to denote the case of $Y = +1$ and blue node the case $Y = -1$. As we can see from Figure 13, the XOR problem is linearly non-separable in the input space. However, if we define a feature mapping $\varphi : \mathbb{R}^2 \mapsto \mathbb{R}^6$ such that

$$(X_1, X_2)^\top \mapsto (X_1^2, X_2^2, \sqrt{2}X_1X_2, \sqrt{2c}X_1, \sqrt{2c}X_2, c)^\top$$

then the XOR problem is linear spearable in $\mathbb{R}^6$ space.

Example 9.2 (Support Vector Machine)**.** Consider a two dimensional feature space contains m data points with binary labels as shown in Figure 14. SVM aims at choosing a separating hyperplane with the maximum geometric margin, which can be expressed as $\rho = \max_{w,b} \min_{i\in[m]} \frac{y_i(w^\top x_i + b)}{||w||_2}$. The equivalent optimizaiton problem can be formalized as

$$\begin{aligned} \underset{w,b}{\text{minimize}} \quad & \frac{1}{2}||w||_2^2 \\ \text{subject to} \quad & y_i(w_i^\top x_i + b) \geq 1,\ \forall i \in [m] \end{aligned}$$

The corresponding KKT conditions include

$$\begin{aligned} & w_i = \sum_{i=1}^m \alpha_i y_i x_i, \quad \sum_{i=1}^m \alpha_i y_i = 0 \\ & \alpha_i [y_i(w^\top x_i + b) - 1] = 0, \quad \forall\ i \in [m] \end{aligned}$$

and the dual problem

$$\begin{aligned} \underset{\alpha}{\text{maximize}} \quad & \sum_{i=1}^m \alpha_i = \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \\ \text{subject to} \quad & \sum_{i=1}^m \alpha_i y_i = 0, \quad \alpha_i \geq 0, \quad \forall\ i \in [m] \end{aligned}$$

Once we solve for the $\alpha_i,\ i \in [m]$, we obtain the linear classifier $f(x) = w^\top x = \sum_{i=1}^m \alpha_i y_i \langle x_i, x \rangle$. We can see from this result that the hypothesis solution only depends on inner products between vectors.

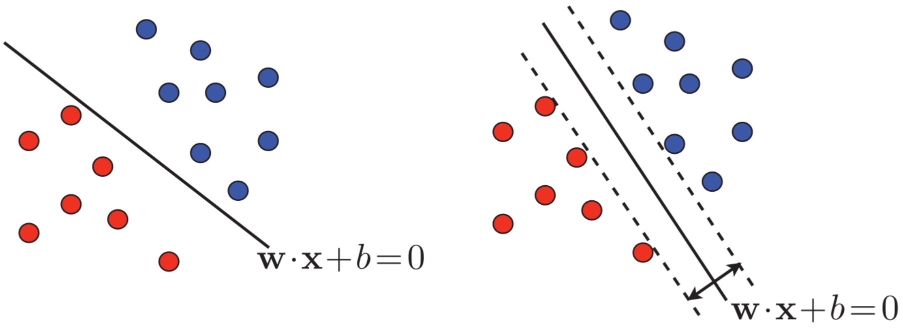

$\mathbf{w}\cdot\mathbf{x}+b=0$
$\mathbf{w}\cdot\mathbf{x}+b=0$

Figure 14: Separating hyperplane

Example 9.3 (Inner Product)**.** Here we illustrate an example of calculating the inner product in feature space $\mathcal{Z}$ instead of originial space $\mathcal{X}$.

$$\begin{aligned} \langle (z_1, z_2, z_3), (z_1', z_2', z_3') \rangle &= \langle \varphi(x_1, x_2), \varphi(x_1', x_2') \rangle \\ &= \langle (x_1^2, \sqrt{2}x_1x_2, x_2^2), (x_1'^2, \sqrt{2}x_1'x_2', x_2'^2) \rangle \\ &= (x_1x_1', x_2x_2')^2 = (\langle x, x' \rangle)^2 \\ &= K(x, x') \end{aligned} \tag{9.1}$$

From the example of SVM, we notice that determining a nonlinear prediction function requires multiple inner product computations in high-dimensional (feature) spaces, which can become very costly. A solution

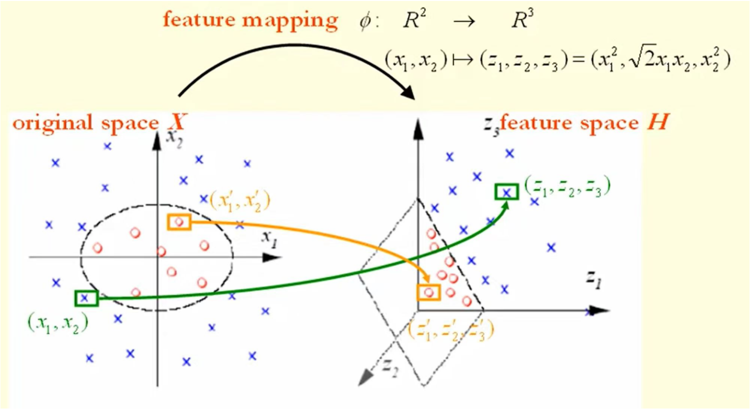


Figure 15: Inner product in feature space

to this problem is to use kernel methods, which are based on kernels or kernel functions. We briefly introduce the concept here and will concretely discuss it in the section of reproducing kernel Hilbert space.

Definition 9.1. A function $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is called a kernel over $\mathcal{X}$.

The idea behind is to define a kernel K such that for any two points $x, x' \in \mathcal{X}$, $K(x, x')$ be equal to an inner product of vectors $\varphi(x)$ and $\varphi(x')$:

$$K(x, x') = \langle \varphi(x), \varphi(x') \rangle \quad \forall\; x, x' \in \mathcal{X}$$

for some features mapping $\varphi : \mathcal{X} \mapsto \mathcal{H}$, where Hilbert space $\mathcal{H}$ is called a feature space. Since an inner product is a measure of the similarity of two vectors, K is often interpreted as a similarity measure between elements of the input space $\mathcal{X}$.

- Distance in feature space $\mathcal{H}$:

$$||\varphi(x) - \varphi(x')||_2^2 = \langle \varphi(x), \varphi(x') \rangle - 2\langle \varphi(x), \varphi(x') \rangle + \langle \varphi(x'), \varphi(x') \rangle = K(x, x) - 2K(x, x') + K(x', x')$$

- Angle in feature space $\mathcal{H}$:

$$\cos\theta = \frac{\langle \varphi(x), \varphi(x') \rangle}{||\varphi(x)||_2 \cdot ||\varphi(x')||_2} = \frac{K(x, x')}{\sqrt{K(x, x) \cdot K(x', x')}}$$

The associated kernel matrix $\mathbf{K}$ is then a matrix of dot-products (Gram matrix), and is thus positive semi-definite, that is, all of its eigenvalues are non-negative, or $\forall\; \alpha^\top \mathbf{K} \alpha \geq 0$. If $\mathcal{H} = \mathbb{R}^d$ and $\Phi \in \mathbb{R}^{n \times d}$ is the matrix of features (or desgin matrix) with i-th row composed of $\varphi(x_i)$, then $\mathbf{K} = \Phi\Phi^\top \in \mathbb{R}^{n \times n}$ is the kernel matrix, while $\frac{1}{n}\Phi^\top\Phi \in \mathbb{R}^{d \times d}$ is the empirical covariance matrix.

Remark 9.1. An important advantage of such a kernel K is efficiency: K is often more efficient to compute than φ and an inner product in $\mathcal{H}$. We will see serveal common examples where the computation of $K(X, X')$ can be achieved in $\mathcal{O}(N)$ while that $\langle \varphi(X), \varphi(X') \rangle$ typically requries $\mathcal{O}(d)$ where d is the dimension of space $\mathcal{H}$, and $d \gg N$.

Perhaps an even more crucial benefit of such a kernel function K is flexibility: there is no need to explicitly define or compute a mapping φ especially when the feature mapping is not always easty to find.

The kenerl K can be arbitrarily chosen so long as the existence of Φ is guaranteed, namely, K satisfies Mercer's condition (we will see in next section).

9.2 Reproducing Kernel Hilbert Space

Many problems in statistics – among them interpolation, regression and density estimation, as well as nonparametric forms of dimension reduction and testing – involve optimizing over function spaces. Hilbert spaces include a reasonably broad class of functions, and enjoy a geometric structure similar to ordinary Euclidean space. A particular class of function-based Hilbert spaces are those defined by reproducing kernels, and these spaces – known as reproducing kernel Hilbert spaces (RKHSs) – have attractive properties from both the computational and statistical points of view.

9.2.1 Hilbert Space

Definition 9.2 (Inner Product)**.** An inner product on a vector space V is a mapping $\langle\cdot,\cdot\rangle_V : V \times V \mapsto R$ such that

$$\begin{aligned} &\langle f,g\rangle_V = \langle g,f\rangle_V && \forall\ f,g \in V \\ &\langle f,g\rangle_V \geq 0, \text{with equality iff } f=0 && \forall\ f \in V \\ &\langle f+\alpha g,h\rangle_V = \langle f,h\rangle_V + \alpha\langle g,h\rangle_V && \forall\ f,g,h \in V, \alpha \in \mathbb{R} \end{aligned} \tag{9.2}$$

A vector space equipped with an inner product is known as an inner product space. Note that any inner product induces a norm via $||f||_V := \sqrt{\langle f,f\rangle_V}$. Given this norm, we can then define the usual notion of Cauchy sequence – that is, a sequence $(f_n)_{n=1}^{\infty}$ with elements in V is Cauchy if, for any $\epsilon > 0$, there exists some integer $\epsilon > 0$, such that there exists some integer $N(\epsilon)$ such that

$$||f_n - f_m||_V < \epsilon \quad \forall\ n,m \geq N(\epsilon)$$

Definition 9.3 (Hilbert Space)**.** A Hilbert space $\mathcal{H}$ is an inner product space $(\langle\cdot,\cdot\rangle_{\mathcal{H}}, \mathcal{H})$ in which every Cauchy sequence $(f_n)_{n=1}^{\infty}$ in $\mathcal{H}$ converges to some element $f^* \in \mathcal{H}$.

A metric space in which every Cauchy sequence $(f_n)_{n=1}^{\infty}$ converges to an element f^* of the space is known as complete. Thus, we can summarize by saying that a Hilbert space is a complete inner product space.

Example 9.4 (Sequence space $l^2(\mathbb{N})$)**.** Consider the space of square-summable real-valued sequences, namely

$$l^2(\mathbb{N}) := \left\{ (\theta_j)_{j=1}^{\infty} \mid \sum_{j=1}^{\infty} \theta_j^2 < \infty \right\}$$

This set, when endowed with the usual inner product $\langle\theta,\gamma\rangle_{l^2(\mathbb{N})}$, defines a classical Hilbert space. It plays an especially important role in our discussion of eigenfunctions for reproducing kernel Hilbert spaces. Note that the Hilbert space $\mathbb{R}^m$, equipped with the usual Euclidean inner product, can be obtained as a finite-dimensional subspace of $l^2(\mathbb{N})$: in particular, the space $\mathbb{R}^m$ is isomorphic to the "slice"

$$\left\{\theta \in l^2(\mathbb{N}) \mid \theta_j = 0,\ \forall j \geq m+1\right\}$$

Example 9.5 (L^2 Space)**.** Any element of the space $L^2[0,1]$ is a function $f : [0,1] \mapsto \mathbb{R}$ that is Lebesgue-integrable, and whose square satisfies the bound

$$||f||_{L^2[0,1]}^2 = \int_0^1 f^2(x)dx < \infty$$

Since this norm does not distinguish between functions that differ only on a set of zero Lebesgue measure, we are implicitly identifying all such functions. The space $L^2[0,1]$ is a Hilbert space when equipped with the inner product

$$\langle f, g\rangle_{L^2[0,1]} = \int_0^1 f(x)g(x)dx$$

In a certain sense, the space $L^2[0,1]$ is equivalent to the sequence space $l^2(\mathbb{N})$. In particular, let $(\phi_j)_{j=1}^{\infty}$ be any complete orthonormal basis of $L^2[0,1]$. By definition, the basis functions satisfy $||\phi_j||_{L^2[0,1]} = 1$ for all $j \in \mathbb{N}$, and $\langle \phi_i, \phi_j\rangle = 0$ for all $i \neq j$, and moreover, any function $f \in L^2[0,1]$ has the representation $f = \sum_{j=1}^{\infty} a_j\phi_j$, where $a_j := \langle f, \phi_j\rangle$ is the j-th basis coefficient. By Parseval's theorem (in Fourier transform), we have

$$||f||_{L^2[0,1]}^2 = \sum_{j=1}^{\infty} a_j^2$$

so that $f \in L^2[0,1]$ if and only if the sequence $a = (a_j)_{j=1}^{\infty} \in l^2(\mathbb{N})$. The correspondence $f \leftrightarrow (a_j)_{j=1}^{\infty}$ thus defines an isomorphism between $L^2[0,1]$ and $l^2(\mathbb{N})$.

9.2.2 Positive Semidefinite Kernel Functions

Let us begin with the notion of a positive semidefinite kernel function. It is a natural generalization of the idea of a positive semidefinite matrix to the setting of general functions.

Definition 9.4 (Positive Semidefinite Kernel Function)**.** A symmetric bivariate function $\mathcal{K} : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is positive semidefinite (PSD) if for all integers $n \geq 1$ and elements $\{x_i\}_{i=1}^n \subset \mathcal{X}$, the $n \times n$ matrix with elements $\mathbf{K}_{ij} := K(x_i, x_j)$ is positive semidefinite.

Example 9.6 (Linear Kernels)**.** When $\mathcal{X} = \mathbb{R}^d$, we can define the linear kernel function $K(x, x') := \langle x, x'\rangle$. It is clearly a symmetric function of its arguments. In order to verify the positive semidefiniteness, let $\{x_i\}_{i=1}^n$ be an arbitrary collection of points in $\mathbb{R}^d$, and consider the matrix $\mathbf{K} \in \mathbb{R}^{n\times n}$ with entries $K_{ij} = \langle x_i, x_j\rangle$. For any vector $\alpha \in \mathbb{R}^n$, we have

$$\alpha^\top \mathbf{K}\alpha = \sum_{i,j=1}^n \alpha_i\alpha_j\langle x_i, x_j\rangle = \left|\left|\sum_{i=1}^n a_i x_i\right|\right|_2^2 \geq 0$$

Since $n \in \mathbb{N}$, $\{x_i\}_{i=1}^n$ and $\alpha \in \mathbb{R}^n$ were all arbitrary, we conclude that K is positive semidefinite kernel.

Example 9.7 (Polynomial Kernels)**.** A natural generalization of the linear kernel on $\mathbb{R}^d$ is the homogeneous polynomial kernel $K(x, z) = (\langle x, z\rangle)^m$ of degree $m \geq 2$, also defined on $\mathbb{R}^d$. Let us demonstrate the positive semidefiniteness of this function in the special case $m = 2$. Note that we have

$$K(x, z) = \left(\sum_{j=1}^d x_j z_j\right)^2 = \sum_{j=1}^d x_j^2 z_j^2 + 2\sum_{i<j} x_i x_j z_i z_j$$

Setting $D = d + \binom{d}{2}$, let us define a mapping $\Phi : \mathbb{R}^d \mapsto \mathbb{R}^D$ with entries

$$\Phi(x) = \begin{bmatrix} x_j^2, & \text{for } j = 1, \ldots, d \\ \sqrt{2} x_i x_j, & \text{for } i < j \end{bmatrix} \tag{9.3}$$

corresponding to all polynomials of degree two in $(x_1, \ldots, x_d)$. With this definition, we see that K can be expressed as a Gram matrix – namely, in the form

$$K(x, z) = \langle \Phi(x), \Phi(z) \rangle_{\mathbb{R}^D}$$

Follow the example of linear kernels, it is straightforward to verify that this Gram representation ensures that K must be positive semidefinite.

An extension of the homogeneous polynomial kernel is the *inhomogeneous* polynomial kernel $K(x, z) = (1 + \langle x, z \rangle)^m$, which is based on polynomials of degree m or less.

Example 9.8 (Gaussian Kernels)**.** As a more exotic example, given some compact subset $\mathcal{X} \subset \mathbb{R}^d$, consider the Gaussian kernel

$$K(x, z) = \exp\left(-\frac{1}{2\sigma^2} ||x - z||_2^2 \right)$$

It is not immediately obvious that K is positive semi-definite.

9.2.3 Constructing an RKHS from a Kernel

9.2.4 Alternative Way to Construct RKHS

9.3 Algorithms

10 Local Averaging Methods

10.1 Quick Review

In empirical risk minmization, our target is to approximate the Bayes predictor by minimizing the expected risk $\mathcal{R}(f) = \mathbb{E}_P[l(Y, f(X))]$. However, the joint distribution of real data $P(X, Y)$ remains unknown, so we have to minimize the empirical risk, which assign uniform weight $1/n$ to each (X_i, Y_i) pair,

$$\hat{f} = \underset{f \in \mathcal{F}}{\arg\min}\ \hat{\mathcal{R}}(f) = \underset{f \in \mathcal{F}}{\arg\min}\ \frac{1}{n}\sum_{i=1}^{n} l(Y_i, f(X_i))$$

In spite of this, the empirical risk is still difficult to optimize as f could be any measurable function. Therefore, in the Section 3, we constrain our choice in a hypothesis space $\mathcal{F}$ in order to make the optimization problem solvable. The two classical cases we consider previously in Section 1 are

- Binary Classification: $\mathcal{Y} = \{-1, 1\}$ with 0-1 loss $l(y, \hat{y}) = \mathbb{1}\{y \neq \hat{y}\}$, then the expected risk is $\mathcal{R}(f) = \mathbb{E}[\mathbb{1}(Y \neq f(X))] = \mathbb{P}(Y \neq f(X))$.
- Regression: $\mathcal{Y} = \mathbb{R}$ with square loss $l(y, \hat{y}) = (y - \hat{y})^2$, and the expected risk $\mathcal{R}(f) = \mathbb{E}[(Y - f(X))^2]$

As seen before, minimizing the expected risk leads to an optimal ”target function”, call the Bayes predictor.

Proposition 10.1 (Bayes Predictor and Bayes Risk)**.** The conditional expected risk is minimized at a Bayes predictor $f^* : \mathcal{X} \to \mathcal{Y}$ satisfying for all $x \in \mathcal{X}$,

$$f^* \in \underset{\text{measurable } f}{\arg\min}\ \mathbb{E}\big[l(Y, f(X))\big]$$

The Bayes risk $\mathcal{R}^*$ is the risk of all Bayes predictors and is equal to

$$\mathcal{R}^* = \inf_{\text{measurable } f} \mathbb{E}\big[l(Y, f(X))\big]$$

Note that the Bayes predictor is not unique, but that all Bayes predictors lead to the same Bayes risk, and that the Bayes risk is usually nonzero (unless the dependence between X and Y is deterministic). Specifially, we have the following special cases:

- Binary Classification: $\mathcal{Y} = \{-1, 1\}$ and $l(y, \hat{y}) = \mathbb{1}\{y \neq \hat{y}\}$, the Bayes predictor is equal to

  $$f^*(X) \in \underset{y \in \{-1,1\}}{\arg\max}\ \mathbb{P}(Y = y \mid X) = \operatorname{sgn}(\eta(X) - 1/2)$$

  where $\eta(X) = \mathbb{P}(Y = 1 \mid X)$ This result extends naturally to multi-category classification with the Bayes predictor

  $$f^*(X) \in \underset{y \in \{1,\ldots,k\}}{\arg\max}\ \mathbb{P}(Y = y \mid X)$$

  Moreover,

  $$\mathcal{R}(f) - \mathcal{R}^* = \mathbb{E}\big[|2\eta(X) - 1| \cdot \mathbb{1}(f^*(X) \neq f(X))\big] \tag{10.1}$$

  This is due to the fact that

  $$\begin{aligned}\mathcal{R}(f) - \mathcal{R}^* &= \mathbb{E}\big[\mathbb{E}[\mathbb{1}(Y \neq f(X)) - \mathbb{1}(Y \neq f^*(X)) \mid X]\big] \\ &= \mathbb{E}\big[\mathbb{E}[\mathbb{1}(1 \neq f(X)) - \mathbb{1}(1 \neq f^*(X)) \mid X, Y = 1] \cdot \eta(X) + \mathbb{E}[\mathbb{1}(-1 \neq f(X)) - \mathbb{1}(-1 \neq f^*(X)) \mid X, Y = -1] \cdot\end{aligned}$$

For any given X, we can look at the two possible cases for the signs of $\eta(x) - 1/2$ and $f(x)$ that lead to different predictions for f and f^*

- $\eta(X) > 1/2$ and $f(X) = -1$, $\mathcal{R}(f) - \mathcal{R}^* = \eta(X) - (1 - \eta(X)) = 2\eta(X) - 1$
- $\eta(X) < 1/2$ and $f(X) = 1$, $\mathcal{R}(f) - \mathcal{R}^* = -\eta(X) + (1 - \eta(X)) = 1 - 2\eta(X)$

- Regression: $\mathcal{Y} = \mathbb{R}$ and $l(y, \hat{y}) = (y - \hat{y})^2$, the Bayes predictor is

$$f^*(X) = \mathbb{E}[Y \mid X]$$

Moreover, with the square loss, we have

$$\begin{aligned}
\mathcal{R}(f) - \mathcal{R}^* &= \mathbb{E}_{X,Y}[l(Y - f(X))] - \mathbb{E}_{X,Y}[l(Y - f^*(X))] \\
&= \int_{\mathcal{X}} \Big\{ \mathbb{E}_Y[(Y - f(X))^2 \mid X = x] - \mathbb{E}_Y[(Y - f^*(X))^2 \mid X = x] \Big\} dP(x) \\
&= \int_{\mathcal{X}} \Big\{ \mathbb{E}_Y\big[2Y(f^*(X) - f(X)) + f(X)^2 - f^*(X)^2 \mid X = x\big] \Big\} dP(x) \\
&= \int_{\mathcal{X}} \Big\{ 2(f^*(x) - f(x))\mathbb{E}_Y[Y \mid X = x] + f(x)^2 - f^*(x)^2 \Big\} dP(x) \\
&= \int_{\mathcal{X}} \Big\{ 2f^*(x)^2 - 2f(x)f^*(x) + f(x)^2 - f^*(x)^2 \Big\} dP(x) \\
&= \int_{\mathcal{X}} \big(f(x) - f^*(x)\big)^2 dP(x) = ||f - f^*||^2_{L_2(\mathbb{P})}
\end{aligned} \tag{10.2}$$

Note that, in general, these relations do not hold for arbitrary loss function.

In a word, empirical risk minimization (ERM) is a method to approximate Bayes predictor f^*, knowing the training samples $S_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ and the loss l, by minimizing the risk or excess risk $\mathcal{R}(f) - \mathcal{R}^*$.

10.2 Local Averaging Methods

Local averaging methods provide a different approach by minimizing the conditional expected risk $\mathbb{E}[l(Y, f(X)) \mid X]$ pointwisely, which leads to the Bayes predictor $f^*(X)$.

Proposition 10.2 (Bayes Predictor and Bayes Risk)**.** The conditional expected risk is minimized at a Bayes predictor $f^* : \mathcal{X} \to \mathcal{Y}$ satisfying for all $x \in \mathcal{X}$,

$$f^*(X) \in \underset{f(X) \in \mathcal{Y}}{\arg\min}\ \mathbb{E}\big[l(Y, f(X)) \mid X\big]$$

The Bayes risk $\mathcal{R}^*$ is the risk of all Bayes predictors and is equal to

$$\mathcal{R}^* = \mathbb{E}_X\Big[\inf_{f(X) \in \mathcal{Y}} \mathbb{E}\big[l(Y, f(X)) \mid X\big]\Big]$$

However, the conditional probability $\mathbb{P}(Y \mid X)$ is generally unknown. To overcome this obstacles, this time we approximate the $\mathbb{P}(Y \mid X)$ by some estimator $\hat{\mathbb{P}}(Y \mid X)$, and the optimal predictor could be obtained by

$$\hat{f}(X) = \underset{f(X) \in \mathcal{Y}}{\arg\min}\ \hat{\mathbb{E}}\big[l(Y, f(X)) \mid X\big] = \underset{f(X) \in \mathcal{Y}}{\arg\min} \int_{\mathcal{Y}} l(y, f(X)) d\hat{P}(Y = y \mid X)$$

which are often called ”plug-in” estimators. Recall what we done in ERM

$$\hat{f} = \arg\min_{f \in \mathcal{F}} \hat{\mathcal{R}}(f) = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} l(Y_i, f(X_i))$$

In the usual cases, local averaging methods leads to the following prediction functions:

- Classification with 0-1 loss:

$$f^*(X) \in \arg\min_{f(X) \in \mathcal{Y}} \hat{\mathbb{E}}\big[\mathbb{1}(Y \neq f(X)) \mid X\big] = \arg\min_{f(X) \in \mathcal{Y}} \sum_{y=1}^{k} \mathbb{1}(y \neq f(X)) \cdot \hat{P}(Y = y \mid X)$$

  which is equivalent to

$$\hat{f}(X) \in \arg\max_{y \in \{1,\ldots,k\}} \hat{P}(Y = y \mid X)$$

- Regression with square loss:

$$\min_{f(X) \in \mathcal{Y}} \int_{\mathcal{Y}} (y - f(X))^2 \; d\hat{P}(Y = y \mid X)$$

  The first-order optimal condition yields

$$\int_{\mathcal{Y}} (2f(X) - 2y) \; d\hat{P}(Y = y \mid X) = 0$$

  which implies

$$\hat{f}(X) = \int_{\mathcal{Y}} y \; d\hat{P}(Y = y \mid X) = \hat{\mathbb{E}}[Y \mid X]$$

In this way, we don’t need to claim a hypothesis on the form of function f, but the tradeoff is we have to estimate the conditional distribution $P(Y \mid X)$ as well as the marginal distribution $P(X)$.

As you shall see later, all of the methods we’re going to introduce in this section can provably learn complex non-linear functions f with a convergence rate of the form $\mathcal{O}(n^{-2/(d+2)})$, where d is the underlying dimension, leading to the curse of dimensionality.

10.3 Linear Estimators

In this section, we will consider ”linear” estimators (which is linear in observations), where the conditional distribution is of the form

$$\hat{P}(Y = y \mid X) = \sum_{i=1}^{n} \hat{w}_i(X) \cdot \mathbb{1}(Y_i = y)$$

with its derviative

$$d\hat{P}(Y = y \mid X) = \sum_{i=1}^{n} \hat{w}_i(X) \cdot \delta_{Y_i}(Y) dy$$

where δ_{Y_i} is the Dirac probability distribution at Y_i, and the weight function $\hat{w}_i : \mathcal{X} \mapsto \mathbb{R}$, $i = 1, \ldots, n$ depends on the input data only (for simplicity) and satisfy for all $i \in \{1, \ldots, n\}$ and $X \in \mathcal{X}$

$$\hat{w}_i(X) \geq 0 \quad \text{and} \quad \sum_{i=1}^{n} \hat{w}_i(X) = 1 \quad \text{almost surely in } X$$

These conditions ensure that for all $x \in \mathcal{X}$, $\hat{P}(Y \mid X)$ is a probability distribution. For our running examples, we have:

- Binary Classification with category labels:

$$\hat{f}(X) \in \underset{y\in\{1,\ldots,k\}}{\arg\max}\ \hat{P}(Y = y \mid X) = \underset{y\in\{1,\ldots,k\}}{\arg\max} \sum_{i=1}^{n} \hat{w}_i(X) \cdot \mathbb{1}(Y_i = y)$$

  that is, each observation (X_i, Y_i) votes for its label with weight $\hat{w}_i(X)$.

- Regression on $\mathcal{Y} = \mathbb{R}$:

$$\hat{f}(X) = \int_{\mathcal{Y}} y \ d\hat{P}(Y = y \mid X) = \sum_{i=1}^{n} \hat{w}_i(X) \int_{\mathcal{Y}} y \cdot \delta_{Y_i}(y) dy = \sum_{i=1}^{n} \hat{w}_i(X) Y_i \tag{10.3}$$

  This is why the terminology ”linear estimators” is sometimes used, since as function of the response vector in $\mathbb{R}^n$, the estimator is linear.

Weight Functions. In most cases, for any i, the weight function $\hat{w}_i(X)$ is closed to 1 for training points X_i which are close to X (measure the similarity with X_i). We next show three classical ways of building them: (1) partition estimators, (2) Nearest-neighbors, and (3) Nadaraya-Waatson estimator (a.k.a. kernel regression).

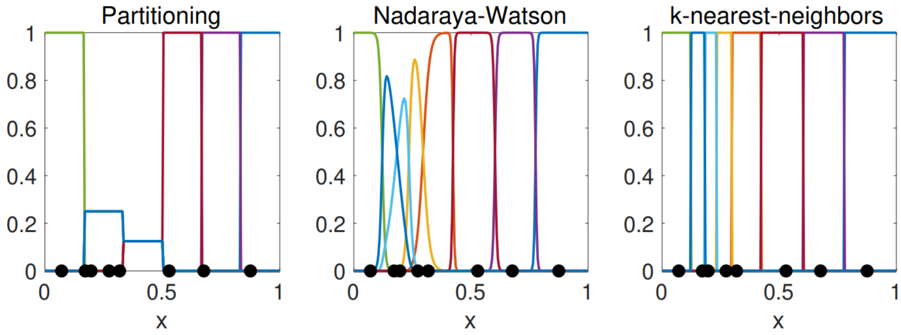


Figure 16: Weights of linear estimators in $d = 1$ estimation for three types of local averaging estimators. The $n = 8$ weight functions $\hat{w}_i(x)$ are plotted with the observations in black.

10.3.1 Partition Estimators

If $\mathcal{X} = \bigcup_{j\in J} A_j$ is a partition (such that for all $j, j' \in J, A_j \cap A_{j'} = \emptyset$) of $\mathcal{X}$ with a countable index set J (which we assume finite for simplicity), then we can conider for any $X \in \mathcal{X}$ the corresponding element $A(X)$ of the partition (namely, $A(X)$ is the unique A_j such that $X \in A_j$), and define

$$\hat{w}_i(X) = \frac{\mathbb{1}_{X_i\in A(X)}}{\sum_{j=1}^{n} \mathbb{1}_{X_j\in A(X)}} \tag{10.4}$$

with the convention that if no training data points $\{X_i\}$ lies in $A(X)$, then $\hat{w}_i(X)$ is equal to $1/n$ for each $i \in \{1, \ldots, n\}$.

Equivalence with Least-squares Regression. Consider the case of regression where we use the linear estimator $\hat{f}(X) = \sum_{i=1}^n \hat{w}_i(X) Y_i$ with partition weights. This can be seen as a least-square estimator with feature vector $\varphi(X) = (\mathbb{1}_{X \in A_1}, \ldots, \mathbb{1}_{X \in A_J})^\top \in \mathbb{R}^J$ in ERM approach. Indeed, from trainning data $(X_1, Y_1), \ldots, (X_n, Y_n)$, we need to find the weight vector $\hat{\theta}$ through the normal equations

$$\sum_{i=1}^n \varphi(X_i)\varphi(X_i)^\top \theta = \sum_{i=1}^n Y_i \varphi(X_i)$$

It turns out that the matrix $\hat{\Sigma} = \sum_{i=1}^n \varphi(X_i)\varphi(X_i)^\top$ is diagonal with the jth component equals to n_{A_j}, the number of data points lying in cell A_j. This implies that for a non-empty cell A_j, θ_j is the average of all Y_i's for X_i lying in A_j, namely,

$$\theta_j = \frac{1}{n_{A_j}} \sum_{i=1}^n Y_i \cdot \mathbb{1}_{X_i \in A_j}$$

Thus, for all $X \in A_j$, the prediction is exactly θ_j, just as the weights obtained from Eq.(10.4). For empty cells, θ_j is not determined. Among the many OLS estimators, we select the one for which the variance of the vector θ is smallest, that is $\sum_{j \in J}(\theta_j - \frac{1}{|J|}\sum_{j' \in J} \theta'_j)^2$ is smallest. A short calculation shows that this exactly leads to $\theta_j = \frac{1}{n}\sum_{i=1}^n Y_i$ for these empty cells, which correspond to our chosen convention.

This equivalence with least-squares estimation with a diagonal (empirical or not) non-centered covariance matrix makes it attractive for theoretical purposes.

Choice of Partitions. These are two standard applications of partition estimators:

- Fixed partitions:

  for example, when $\mathcal{X} = [0,1]^d$, then we choose the bandwidth h, with $|J| = h^{-d}$ (if $h = 1/5$ and $d = 2$, we have $|J| = 25$). Note here that the computation time for ech $X \in \mathcal{X}$ is not necessarily proportional to $|J|$, but to n (by simply considering the bins where the data lie). This estimator is some times called a ”regressogram”.

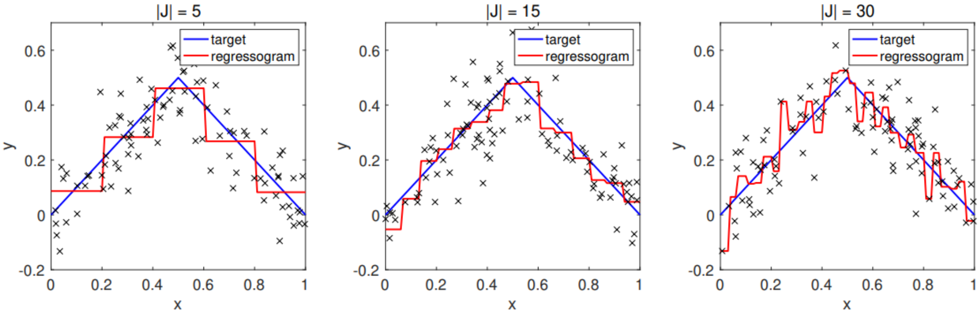


Figure 17: Regressograms in $d = 1$ dimension, with three different values of $|J|$. We can see both underfitting, or overfitting in this example. Note that the target function f^* is piecewise affine, and that on the affine parts, the estimator is far from linear, namely, the estimator cannot take advantage of extra-regularity.

- Decision trees:

  for data in a hypercube, we can recursively partition it by selecting a variable to split leading to a maximum reduction in errors when defining the partitioning estimate. Note that now the partition depends on the labels (so the analysis below does not apply, unless the partitioning is learned on a different data than the one sued for the estimation).

10.3.2 Nearest-Neighbors

Given an integer $k \geq 1$, and a distance d on $\mathcal{X}$, for any $X \in \mathcal{X}$, we can order the n samples so that

$$d(X_{i_1(X)}, X) \leq d(X_{i_2(X)}, X) \leq \cdots \leq d(X_{i_n(X)}, X)$$

where $\{i_1(X), \ldots, i_n(X)\} = \{1, \ldots, n\}$, and ties are broken randomly. We then define

$$\hat{w}_i(X) = \frac{1}{k}, \quad \text{if } i \in \{i_1(X), \ldots, i_k(X)\}$$

and $\hat{w}_i(X) = 0$ otherwise. Given a new input $X \in \mathcal{X}$, the nearest-neighbors predictor looks at the k nearest points X_i in the data set $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ and predicts a majority vote among them for classification or simply the averaged response for regression. The number of nearest neighbors k is a hyperparameter which needs to be estimated (typically by cross-validation).

Algorithms. Given a test point $X \in \mathcal{X}$, the naive algorithm looks at all training data points for computing the predicted response, thus the complexity is $O(nd)$ per test point in $\mathbb{R}^d$. When n is large, this is costly in time and memory. There exists indexing techniques for (potentially approximate) nearest-neighbor search, such as "k-dimensional-trees", with typically a logarithmic complexity in n (but with some additional compiling time).

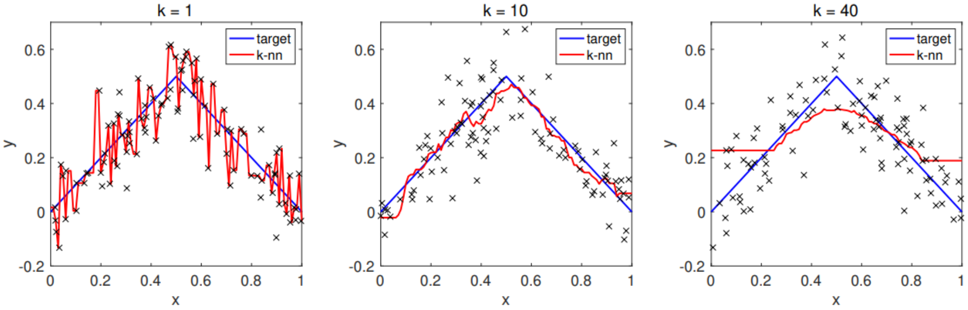


Figure 18: k-nearest neighbor regression in $d = 1$ dimension, with three values of k (the number of neighbors). We can see both underfitting (k too large), and overfitting (k too small).

10.3.3 Nadaraya-Watson Estimator (Kernel Regression)

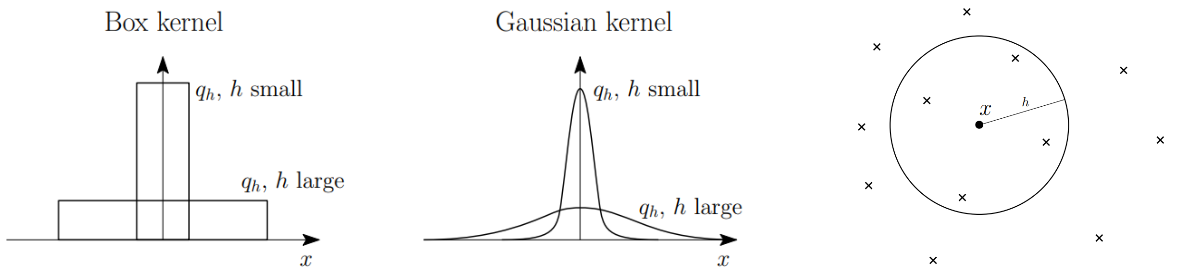
Given a "kernel" function $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}_+$, which is pointwise non-negative, we define

$$\hat{w}_i(X) = \frac{K(X_i, X)}{\sum_{j=1}^n K(X_j, X)}$$

with the convention that if $K(X_j, X) = 0$ for all $j \in \{1, \ldots, n\}$, then $\hat{w}_i(X)$ is equal to $1/n$ for each i. In most case where $\mathcal{X} \subset \mathbb{R}^d$, we take

$$K(X, X') = \frac{q((X - X')/h)}{h^d}$$

for a certain function $q : \mathbb{R}^d \mapsto \mathbb{R}_+$ that has large values around 0, and $h > 0$ a bandwidth parameter to be selected. If we assume that q is integrable with integral equal to one, then $K(\cdot, X')$ is a probability density with mass around X', which gets more concentrated as h goes to zero. See illustration below for the two typical windows.



(a) Two typical kernel windows

(b) Box kernel in $d = 2$ dimensions

- Box kernel: $q(X) = \mathbb{1}(||X||_2 \leq 1)$. See above for an illustration in $d = 2$ dimension
- Gaussian kernel: $q(X) = e^{-||X||^2/2}$, where we use the fact it is non-negative pointwise (as opposed to positive definitiness).

In terms of algorithms, with a naive algorithm, for every test point, all the input data have to be considered, that is, a complexity proportional to n. The same techniques used for efficient k-nearest-neighbor search (e.g. k-d-tress) can be applied here as well.

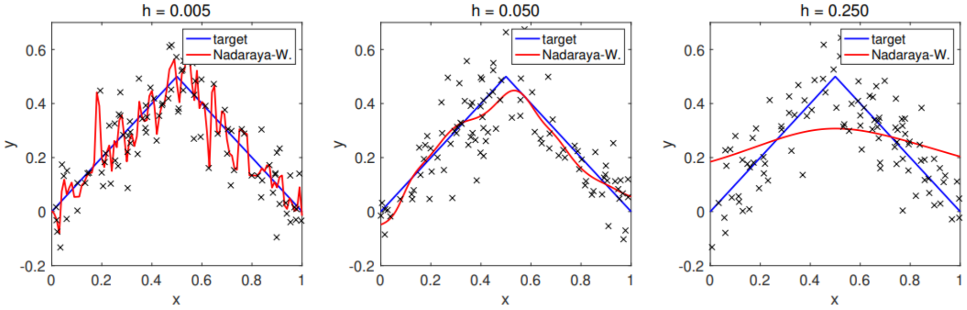


Figure 20: Nadaraya-Watson regression in $d = 1$ dimension, with three values of bandwidth h for the Gaussian kernel.

10.4 Generic Consistency Analysis

We consider for simplicity the **regression** case. For classification, calibration techniques such as those used in Section 2 can be used (with then a square root calibration function on top of the least-squares excess risk), but better rate can be obtained directly (please refer the book Bach 2021).

Except for the requirement of square-integrable for target function $f(x)$, we make extra generic assumptions here:

1. **Bounded noise**: there exists $\sigma \geq 0$ such that $|Y - \mathbb{E}[Y \mid X]|^2 \leq \sigma^2$ almost surely.
2. **Regular target function**: the target function $f^*(x) = \mathbb{E}[Y \mid X = x]$ is B-Lipschitz-continuous with respect to a distance d.

Recall the target function $f^*(x) = \mathbb{E}[Y \mid X = x]$ and the predictor $\hat{f}(x) = \sum_{i=1}^n \hat{w}_i(x) \cdot Y_i$ in Eq.(10.3) at a test point $x \in \mathcal{X}$. Using that the summation of weights $w_i(X)$ is one, we have:

$$\begin{aligned}
\hat{f}(x) - f^*(x) &= \sum_{i=1}^n \hat{w}_i(x) \cdot Y_i - \mathbb{E}[Y \mid X = x] \\
&= \sum_{i=1}^n \hat{w}_i(x) \cdot (Y_i - \mathbb{E}[Y_i \mid X_i]) + \sum_{i=1}^n \hat{w}_i(x) \cdot (\mathbb{E}[Y_i \mid X_i] - \mathbb{E}[Y \mid X = x]) \\
&= \underbrace{\sum_{i=1}^n \hat{w}_i(x) \cdot (Y_i - \mathbb{E}[Y_i \mid X_i])}_{\text{part I}} + \underbrace{\sum_{i=1}^n \hat{w}_i(x) \cdot (f^*(X_i) - f^*(x))}_{\text{part II}}
\end{aligned}$$

Conditioning on $X_1, \ldots, X_n$ and because we have assumed the weight functions do not depend on the labels $\{Y_i\}$, the first term (part I) has zero expectation (with respect to sample S_n)

$$\begin{aligned}
\mathbb{E}_{S_n}\Big[\text{part I} \mid X_1, \ldots, X_n\Big] &= \hat{w}_i(x) \cdot \mathbb{E}\big[Y_i - \mathbb{E}[Y \mid X_i] \mid X_i\big] \\
&= \hat{w}_i(x) \cdot \big(\mathbb{E}[Y_i \mid X_i] - \mathbb{E}[Y_i \mid X_i]\big) = 0
\end{aligned}$$

while the second term (part II) is deterministic and the variance is therefore zero

$$\operatorname*{Var}_{S_n}\Big(\text{part II} \mid X_1, \ldots, X_n\Big) = 0$$

We thus have, using the independencies of samples $(X_i, Y_i).i = 1, \ldots, n$ and weights $w_i(x)$ sum to one:

$$\begin{aligned}
\mathbb{E}_{S_n}\left[\Big(\hat{f}(x) - f^*(x)\Big)^2 \mid X_1, \ldots, X_n\right] &= \Big(\mathbb{E}_{S_n}\Big[\hat{f}(x) - f^*(x) \mid X_1, \ldots, X_n\Big]\Big)^2 + \operatorname*{Var}_{S_n}\Big(\hat{f}(x) - f^*(x) \mid X_1, \ldots, X_n\Big) \\
&= \Big(\mathbb{E}_{S_n}\Big[\text{part II} \mid X_1, \ldots, X_n\Big]\Big)^2 + \operatorname*{Var}_{S_n}\Big(\text{part I} \mid X_1, \ldots, X_n\Big) \\
&= \underbrace{\left(\sum_{i=1}^n \hat{w}_i(x) \cdot \big(f^*(X_i) - f^*(x)\big)\right)^2}_{\text{bias}} + \underbrace{\sum_{i=1}^n \hat{w}_i(x)^2 \cdot \mathbb{E}_{S_n}\Big[\big(Y_i - \mathbb{E}[Y_i \mid X_i]\big)^2 \mid X_i\Big]}_{\text{variance}}
\end{aligned}$$

with a "bias" term which is zero if f^* is constant over $\mathcal{X}$, and a "variance" term which is zero, when Y is a deterministic function of X. We can further bound these as

$$\begin{aligned}
\mathbb{E}_{S_n}\left[\Big(\hat{f}(x) - f^*(x)\Big)^2 \mid X_1, \ldots, X_n\right] &\leq \left(\sum_{i=1}^n \hat{w}_i(x) \cdot \Big|f^*(x_i) - f^*(x)\Big|\right)^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \quad \text{(Assumption 1)} \\
&\leq \left(\sum_{i=1}^n \hat{w}_i(x) \cdot B \cdot d(X_i, x)\right)^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \quad \text{(Assumption 2)} \\
&\leq B^2 \sum_{i=1}^n \hat{w}_i(x) \cdot d(X_i, x)^2 + \sigma^2 \sum_{i=1}^n \hat{w}_i(x)^2 \quad \text{(Jensen's inequality)}
\end{aligned} \tag{10.5}$$

According to Eq.(10.2), the expected excess risk for regression case is:

$$\begin{aligned}\mathcal{R}(\hat{f})-\mathcal{R}^* &= \mathbb{E}\left[l(Y,\hat{f}(x))-l(Y,f^*(x))\right]\\ &= \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\left(\hat{f}(x)-f^*(x)\right)^2 \mid X=x\right]dP(x)\\ &\le \underbrace{B^2\int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^n \hat{w}_i(x)d(X_i,x)^2\right]dP(x)}_{\text{bias term}}+\underbrace{\sigma^2\int_{\mathcal{X}}\mathbb{E}_{S_n}\left[\sum_{i=1}^n \hat{w}_i(x)^2\right]dP(x)}_{\text{variance term}}\end{aligned}\tag{10.6}$$

Notice that the expectation is with respect to the training data S_n, where the expectation with respect to the testing point X is kept as an integral to avoid confusions. This upper bound can be divided into:

- A bias term $B^2\int_{\mathcal{X}}\mathbb{E}\left[\sum_{i=1}^n \hat{w}_i(x)d(X_i,x)^2\right]dP(x)$, which depends on the regularity of the target function.
- A variance term $\sigma^2\sum_{i=1}^n\int_{\mathcal{X}}\mathbb{E}\left[\hat{w}_i(x)^2\right]dP(x)$, that depends on the noise on top of the optimal predictions. Since the weights sum to one, we can write

  $$\sum_{i=1}^n \mathbb{E}[\hat{w}_i(x)^2]=\sum_{i=1}^n \mathbb{E}[(\hat{w}_i(x)-1/n)^2]+2/n-1/n^2$$

  Hence, up to vanishing constant, the variance term measures the deviation t0 the uniform weights.

Both variance and bias have to go to zero when n grows, and this corresponds to two simple quantities on the weights. For the variance, the worst case scenario is that $\hat{w}_i(X)^2\approx\hat{w}_i(X)$, that is, weights are putting all the mass in to a single label (different for different testing sample), thus leading to overfitting. For the bias, the worst case scenario is that weights are uniform (the distance $d(X_i,X)$ are different, may lead to underfitting).

10.4.1 Fixed Partition

Proposition 10.3 (Convergence rate for partition estimates)**.** Assume bounded noise (A1) and a Lipschitz-continuous target function (A2), and a partition $\mathcal{X}=\bigcup_{j\in J}A_j$; then for the partitioning estimate $\hat{f}$, we have

$$\int_{\mathcal{X}}\mathbb{E}_{S_n}\left[\left(\hat{f}(x)-f^*(x)\right)^2\right]dP(x)\le\left(8\sigma^2+\frac{B^2}{2}\mathrm{diam}(\mathcal{X})^2\right)\frac{|J|}{n}+B^2\max_{j\in J}\mathrm{diam}(A_j)^2\tag{10.7}$$

where the diameter of set $\mathcal{X}$ is defined as $\mathrm{diam}(\mathcal{X})=\sup\{d(x,x')\mid x,x'\in\mathcal{X}\}$.

There is a tradeoff between bias and variance, and we need to balance the terms (up to constants) $\max_{j\in J}\mathrm{diam}(A_j)^2$ and $|J|/n$. Consider the case of unit-cube $[0,1]^d$, with $|J|=h^{-d}$ cubes of length h, we have $|J|/n\approx 1/(nh^d)$ and $\max_{j\in J}\mathrm{diam}(A_j)^2\approx h^2$, which are equal when $h\approx n^{-1/(2+d)}$, leads to a rate proportional to $n^{-2/(2+d)}$.

While optimal, this is a very slow rate, and a typical example of the curse of dimensionality. For this rate to be small, n has to be exponentially large in dimension. This is unavoidable with so little regularity (only bounded first-order derivatives). In Section 9, we show how to leverage smoothness to get significantly improved bounds. In Section 11, we will leverage dependence on a small number of variables.

Proof. We consider an element A_j of the partition with at least one observation in it (a non-empty cell).

Then for the test point $x \in A_j$ and i among the indices of training points lying in A_j, we have

$$\hat{w}_i(x) = 1/n_{A_j}$$

where $n_{A_j} \in \{1, \ldots, n\}$ is the number of data points lying in A_j.

- **Variance**. From Eq.(10.6), the variance term is bounded from above by σ^2 times

  $$\sum_{i=1}^{n} \hat{w}_i(x)^2 = n_{A_j} \frac{1}{n_{A_j}^2} = \frac{1}{n_{A_j}}$$

  If A_j contains no input observations, then all weights are equal to $1/n$ and this sum is equal to $n \times (1/n^2) = 1/n$ for all $X \in A_j$. Thus we get

  $$\begin{aligned} \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)^2\right] dP(x) &= \int_{\mathcal{X}} \sum_{j\in J} \mathbb{1}(x \in A_j) \cdot \mathbb{E}_{S_n}\left[\frac{1}{n_{A_j}}\mathbb{1}(n_{A_j} > 0) + \frac{1}{n}\mathbb{1}(n_{A_j} = 0)\right] dP(x) \\ &= \sum_{j\in J} \mathbb{P}(A_j) \cdot \mathbb{E}_{S_n}\left[\frac{1}{n_{A_j}}\mathbb{1}(n_{A_j} > 0) + \frac{1}{n}\mathbb{1}(n_{A_j} = 0)\right] \end{aligned} \tag{10.8}$$

  Intuitively, by the law of large numbers, n_{A_j}/n tends to $\mathbb{P}(A_j)$, so the variance term is expected to be of the order $\sigma^2 \sum_{j\in J} \mathbb{P}(A_j)\frac{1}{n\mathbb{P}(A_j)} = \sigma^2 \frac{|J|}{n}$, which is to be expected as this is essentially equivalent to the least-squares regression with features $(\mathbb{1}(X \in A_j))_{j\in J}$.

  More formally, we have $\mathbb{P}(n_{A_j} = 0) = (1 - \mathbb{P}(A_j))^n$. Using Bernstein's inequality for the random variable $\mathbb{1}(X \in A_j)$, which have mean and variance upper-bounded by $\mathbb{P}(A_j)$ (namely, $\mu, \sigma^2 \le \mathbb{P}(A_j)$), we have

  $$\begin{aligned} \mathbb{P}\left(\frac{n_{A_j}}{n} \le \frac{\mathbb{P}(A_j)}{2}\right) &= \mathbb{P}\left(\frac{n_{A_j}}{n} - \mathbb{P}(A_j) \le -\frac{\mathbb{P}(A_j)}{2}\right) \\ &\le \mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n} \mathbb{1}(X_i \in A_j) - \mathbb{E}[\mathbb{1}(X \in A_j)]\right| \ge \frac{\mathbb{P}(A_j)}{2}\right) \\ &\le \exp\left(-\frac{n\mathbb{P}(A_j)^2/4}{2\mathbb{P}(A_j) + 2(\mathbb{P}(A_j)/2)/3)}\right) \\ &\le \exp\left(-\frac{n\mathbb{P}(A_j)}{10}\right) \le \frac{5}{n\mathbb{P}(A_j)} \end{aligned}$$

  where the last inequality holds by knowing the fact that $e^{-x} \le 1/(2x)$ when $x > 0$. Such result leads to the bound

  $$\begin{aligned} &\sum_{j\in J} \mathbb{P}(A_j) \cdot \mathbb{E}_{S_n}\left[\frac{1}{n_{A_j}}\mathbb{1}(n_{A_j} > 0) + \frac{1}{n}\mathbb{1}(n_{A_j} = 0)\right] \\ &= \sum_{j\in J} \mathbb{P}(A_j) \cdot \mathbb{E}_{S_n}\left[\frac{1}{n_{A_j}}\mathbb{1}(n_{A_j} > 0) \cdot \left(\mathbb{1}\left(n_{A_j} \le \frac{n\mathbb{P}(A_j)}{2}\right) + \left(n_{A_j} > \frac{n\mathbb{P}(A_j)}{2}\right)\right) + \frac{1}{n}\mathbb{1}(n_{A_j} = 0)\right] \\ &\le \sum_{j\in J} \mathbb{P}(A_j) \cdot \left[\mathbb{P}\left(\frac{n_{A_j}}{n} \le \frac{\mathbb{P}(A_j)}{2}\right) + \frac{2}{n\mathbb{P}(A_j)} + \frac{1}{n}\mathbb{P}(n_{A_j} = 0)\right] \\ &\le \sum_{j\in J} \mathbb{P}(A_j) \cdot \left[\frac{5}{n\mathbb{P}(A_j)} + \frac{2}{n\mathbb{P}(A_j)} + \frac{1}{n\mathbb{P}(A_j)}\right] \le \frac{8|J|}{n} \end{aligned}$$

- **Bias**. We have, for $X \in A_j$ and a non-empty cell A_j,

$$\sum_{i=1}^{n} \hat{w}_i(X) d(X_i, X)^2 \leq \mathrm{diam}(A_j)^2$$

and $\sum_{i=1}^{n} \hat{w}_i d(X_i, X)^2 = \frac{1}{n} \sum_{i=1}^{n} d(X_i, X)^2 \leq \mathrm{diam}(\mathcal{X})^2$ from empty-cells. Thus, separating the cases $n_{A_j} = 0$ and $n_{A_j} > 0$:

$$\begin{aligned}
\int_{\mathcal{X}} \mathbb{E}_{S_n} \left[\sum_{i=1}^{n} \hat{w}_i(x) d(X_i, x)^2 \right] dP(x) &= \int_{\mathcal{X}} \sum_{j \in J} \mathbb{1}(x \in A_j) \cdot \mathbb{E}_{S_n} \left[\sum_{i=1}^{n} \hat{w}_i(x) d(X_i, x)^2 \right] dP(x) \\
&\leq \int_{\mathcal{X}} \sum_{j \in J} \mathbb{1}(x \in A_j) \cdot \mathbb{E}_{S_n} \Big[\mathrm{diam}(A_j)^2 \cdot \mathbb{1}(n_{A_j} > 0) + \mathrm{diam}(\mathcal{X})^2 \cdot \mathbb{1}(n_{A_j} = 0) \Big] dP(x) \\
&= \sum_{j=1}^{J} \mathbb{P}(A_j) \cdot \Big[\mathrm{diam}(A_j)^2 \cdot \mathbb{P}(n_{A_j} > 0) + \mathrm{diam}(\mathcal{X})^2 \cdot \mathbb{P}(n_{A_j} = 0) \Big] \\
&\leq \sum_{j=1}^{J} \mathbb{P}(A_j) \cdot \Big[\mathrm{diam}(A_j)^2 + \mathrm{diam}(\mathcal{X})^2 \cdot \big(1 - \mathbb{P}(A_j)\big)^n \Big] \\
&\leq \sum_{j=1}^{J} \mathbb{P}(A_j) \cdot \Big[\mathrm{diam}(A_j)^2 + \mathrm{diam}(\mathcal{X})^2 \cdot \frac{1}{2n\mathbb{P}(A_j)} \Big] \qquad (1) \\
&= \sum_{j \in J} \mathbb{P}(A_j) \cdot \mathrm{diam}(A_j)^2 + \frac{|J|}{2n} \cdot \mathrm{diam}(\mathcal{X})^2 \\
&\leq \max_{j \in J} \mathrm{diam}(A_j)^2 + \frac{|J|}{2n} \cdot \mathrm{diam}(\mathcal{X})^2
\end{aligned}$$

The inequality (1) holds because of the fact that $(1-x)^n \leq 1/(2nx)$ for $x \in (0, 1]$.

Combining the upper-bounds of variance and bias term together leads to the desire results.

□

10.4.2 K-nearest Neighbors

In this case, we immediately have $\sum_{i=1}^{n} \hat{w}_i(x)^2 = 1/k$, so the variance term in Eq.(10.6) will go down as soon as k tends to infinity. For the bias term, the needed term $\sum_{i=1}^{n} \hat{w}_i(x) d(X_i, x)^2$ is equal to the average squared distances between test point X and its k-nearest neighbors with training samples $\{X_1, \ldots, X_n\}$, and this is less than the expected distance to the k-nearest neighbor, for which the two following lemmas give an estimate for the l_∞-distance, and thus for all distances by equivalence of norms on $\mathbb{R}^d$.

Lemma 10.1 (Distance to nearest neighbor)**.** Consider a probability distribution with compact support in $\mathcal{X} \subset \mathbb{R}^d$. Consider $n+1$ points $X_1, \ldots, X_n, X_{n+1}$ sampled i.i.d. from $\mathcal{X}$. Then the **expected** squared l_∞-distance between X_{n+1} and its first-nearest-neighbor is less than

$$4 \frac{\mathrm{diam}(\mathcal{X})^2}{n^{2/d}}$$

for $d \geq 2$, and less than $\frac{2}{n} \mathrm{diam}(\mathcal{X})^2$ for $d = 1$.

Proof. By symmetry, we aim at computing the value $\frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{E}[||X_i - X_{(i)}||_\infty^2]$, where $X_{(i)}$ is a nearest neighbor of X_i among the other n points. Denote $R_i = ||X_i - X_{(i)}||_\infty$, then the sets $B_i = \{X \in \mathbb{R}^d \mid$

$||X - X_i||_\infty < R_i/2\}$ are disjoint.

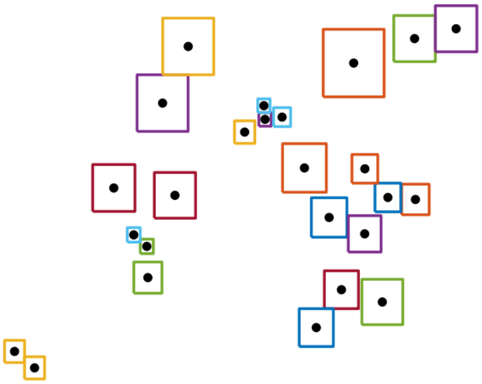


Figure 21: Distance to nearest neighbors

Moreover, their union has diameter less than $\text{diam}(\mathcal{X}) + \text{diam}(\mathcal{X}) = 2\text{diam}(\mathcal{X})$. Thus by comparing volumes, we have: $\sum_{i=1}^{n+1} R_i^d \leq (2\text{diam}(\mathcal{X}))^d$. Therefore, by Jensen's inequality, for $d \geq 2$,

$$\left(\frac{1}{n+1}\sum_{i=1}^{n+1} R_i^2\right)^{d/2} \leq \frac{1}{n+1}\sum_{i=1}^{n+1}(R_i)^d \leq \frac{2^d\text{diam}(\mathcal{X})^d}{n+1}$$

leading to the desired result. For $d = 1$, we simply have

$$\left(\frac{1}{n+1}\sum_{i=1}^{n+1} R_i^2\right) \leq \text{diam}(\mathcal{X})\left(\frac{1}{n+1}\sum_{i=1}^{n} R_i\right) \leq \frac{2}{n+1}\text{diam}(\mathcal{X})^2$$

□

Lemma 10.2 (Distance to k-nearest neighbor)**.** Let $k \geq 1$. Consider a probability distribution with compact support in $\mathcal{X} \subset \mathbb{R}^d$. Consider $n+1$ points $X_1, \ldots, X_n, X_{n+1}$ sampled i.i.d. from $\mathcal{X}$. Then the expected squared l_∞-distance between X_{n+1} and its k-nearest neighbor is less than

$$8\text{diam}(\mathcal{X})^2\left(\frac{2k}{n}\right)^{2/d}$$

for $d \geq 2$, and less than $\text{diam}(\mathcal{X})^2\frac{2k}{n}$ for $d = 1$.

Proof. Without loss of generality, we assume $2k \leq n$ (otherwise, the bound is trivial).

see textbook

□

Proposition 10.4 (Convergence rate for k-nearest neighbors)**.** Assume bounded noise (A1) and a B-Lipchitz-continuous target function $(A2)$. Then for the k-nearest neighbor estimate $\hat{f}$ with the l_∞-norm, we have, for $d \geq 2$

$$\int_{\mathcal{X}} \mathbb{E}_{S_n}\left[(\hat{f}(x) - f^*(x))^2\right] dP(x) \leq \frac{\sigma^2}{k} + 8B^2\text{diam}(\mathcal{X})^2\left(\frac{2k}{n}\right)^{2/d} \tag{10.9}$$

Balancing the two terms above is obtained with $k \approx n^{2/(2+d)}$, and we obtain the same result as for the other local averaging schemes.

10.4.3 Kernel Regression

In this section, we assume that $\mathcal{X} = \mathbb{R}^d$, and for simplicity, we assume that marginal distribution $P(x)$ has a density $p(x)$ with respect to the Lebesgue measure. We also assume that

$$K(X, X') = q_h(X - X') = \frac{q((X - X')/h)}{h^d}$$

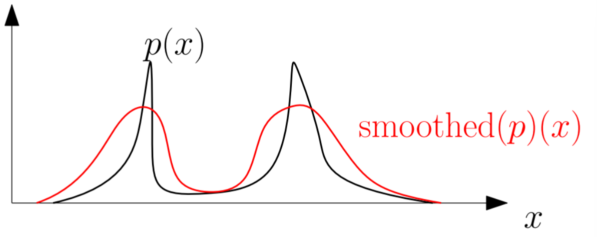
for a probability desntiy $q : \mathbb{R}^d \mapsto \mathbb{R}_+$. The function q_h is also a density, which is the density of hZ when random variable Z has density $q(Z)$ (it is thus gets more concentrated around 0 as h tends to zero). With these notations, the weights can be written as

$$\hat{w}_i(x) = \frac{K(X_i, x)}{\sum_{j=1}^n K(X_j, x)} = \frac{q_h(x - X_i)}{\sum_{j=1}^n q_h(x - X_j)}$$

Smoothing by convolution. When performing kernel smoothing, quantities like $\frac{1}{n}\sum_{i=1}^n q_h(x - X_i)g(X_i)$ naturally appear. When the number n of observations goes to infinity, by the law of large numbers, it tends to almost surely to

$$\int_{\mathbb{R}^d} q_h(X - z)g(z)p(z)dz$$

which is exactly the convolution between the function q_h and the function $x \mapsto p(x)g(x)$, which we can denote $q_h * (pg)(x)$. The function q_h is a probability density that is putting all most its weights at range of values which are of order h, e.g., for kernels like the Gaussian kernel or the box kernel. Thus convolution will smooth the function pg by averaging values which are at range h. Thus, when h goes to zero, it converges to the function pg itself (note that for this limit to hold, we need to make sure the factors in n and h^d are present). See an example below for $g = 1$.



We can now look at the generalization bound from Eq.(10.6) and see how it applies to kernel regression. We now consider the l_2-distance for simplicity, and consider the variance and bias term separately, first with an asymptotic result and then a formal result.

Variance term. We have, for a fixed test point $x \in \mathcal{X}$:

$$n\sum_{i=1}^n \hat{w}_i(x)^2 = \frac{\frac{1}{n}\sum_{i=1}^n q_h(x - X_i)^2}{\left(\frac{1}{n}\sum_{i=1}^n q_h(x - X_i)\right)^2}$$

Using the law of large numbers and the smoothing reasoning above, this summation $n\sum_{i=1}^n \hat{w}_i(x)^2$ is converging almost surely to the mean

$$\frac{\int_{\mathbb{R}^d} q_h(x - z)^2 p(z)dz}{\left(\int_{\mathbb{R}^d} q_h(x - z)p(z)dz\right)^2} = \frac{q_h^2 * p(x)}{(q_h * p(x))^2}$$

When h tends to zero, then the denominator above $(q_h * p(x))^2$ tends to $p(x)^2$ because the bandwidth of the smoothing goes to zero ($q_h \to \delta(x)$). The numerator above corresponds to the smoothing of p by the density $x \mapsto \frac{q_h(x)^2}{\int_{\mathbb{R}^d} q_h(u)^2 du}$ (where $\int_{\mathbb{R}^d} q_h(u)^2 du$ here is just a normalize constant), and is thus asymptotically equivalent to

$$q_h^2 * p(x) \to p(x) \int_{\mathbb{R}^d} q_h(u)^2 du = p(x) h^{-d} \int_{\mathbb{R}^d} q(u)^2 du$$

where $q_h(X - X') = \frac{q((X-X')/h)}{h^d}$. Overall, when n tends to infinity, and h tends to zero, we get:

$$\sum_{i=1}^n \hat{w}_i(x)^2 \sim \frac{1}{nh^d} \frac{1}{p(x)} \int_{\mathbb{R}^d} q(u)^2 du$$

and thus

$$\int_{\mathcal{X}} \left[\sum_{i=1}^n \hat{w}_i(x)^2 \right] p(x) dx \sim \frac{1}{nh^d} \mathrm{vol}(\mathrm{supp}(P)) \int_{\mathcal{R}^d} q(u)^2 du$$

Bias term. With the same intuitive reasoning, we get, when n tends to infinity:

$$\sum_{i=1}^n \hat{w}_i(x) d(X_i, x)^2 \to \frac{\int_{\mathcal{R}^d} q_h(x-z) ||x-z||_2^2 p(z) dz}{\int_{\mathbb{R}^d} q_h(x-z) p(z) dz}$$

The denominator has the same shape for the variance term and tends to $p(x)$ when h tends to zero. With the change of variable $u = \frac{1}{h}(x-z)$, the numerator is equal to

$$\int_{\mathbb{R}^d} q_h(x-z) ||x-z||_2^2 p(z) dz = h^2 \int_{\mathbb{R}^d} q(u) ||u||_2^2 p(x - hu) du$$

which is equivalent to $h^2 p(x) \int_{\mathbb{R}^d} q(u) ||u||_2^2 du$ when h tends to zero. Overall, when n tends to infinity, and h tends to zero, we get:

$$\int_{\mathcal{X}} \left[\sum_{i=1}^n \hat{w}_i(x) d(X_i, x)^2 \right] p(x) dx \sim h^2 \int_{\mathbb{R}^d} q(u) ||u||_2^2 du$$

Overall result. Combining the results from variance and bias terms, we get an *asymptotic bound* of Eq.(10.6) proportional to (up to constants depending on q):

$$\frac{\sigma^2}{nh^d} + B^2 h^2$$

leading to the same upper-bound as for partitioning estimates, by setting $h \approx n^{-1/(d+2)}$.

We can make the informal reasoning above more formal using concentration inequalities, leading to non-asymptotic bounds of the same nature (simply more complicated), that make explicit the joint dependence on n and h.

Proposition 10.5 (Convergence rate for Nadaraya-Watson estimation)**.** Assume bounded noise (A1) and a Lipschitz-continuous target function (A2), and a function $q : \mathbb{R}^d \mapsto \mathbb{R}$ such that $\int_{\mathbb{R}^d} q(z) dz = 1$, and $||q||_\infty = \sup_{z \in \mathbb{R}^d} q(z)$ is finite. We also assume that $p(x) \in [p_{\min}, p_{\max}]$ for all $x \in \mathcal{X}$. Then for the

Nadaraya-Watson estimate $\hat{f}$, we have:

$$\mathcal{R}(\hat{f}) - \mathbb{R}^* = \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[(\hat{f}(X) - f^*(X)) \mid X = x \right] dP(x) \leq \frac{4||q||_\infty}{p_{\min}} \cdot \frac{2\sigma^2 + B\text{diam}(\mathcal{X})^2}{nh^d} + 2h^2 \cdot \frac{p_{\max}}{p_{\min}} \int_{\mathcal{R}^d} q(u)||u||_2^2 du \tag{10.10}$$

Before giving the proof, we note that the optimal bandwidth parameter is indeed proportional to $h \approx n^{-1/(d+2)}$, with an overall excess risk proportional to $n^{-2/(d+2)}$.

Proof. In order to deal with the denominator in the definition of the weights, we can firstly use Bernstein's inequality, applied to the random variables $q_h(X - X_i)$ which is almost surely in $[0, h^{-d}||q||_\infty]$, to bound

$$\mathbb{P}\left(\frac{1}{n} \sum_{i=1}^{n} q_h(X - X_i) \leq \mathbb{E}_Z[q_h(X - Z) - \varepsilon] \right) \leq \exp\left(-\frac{n\varepsilon^2}{2\mathbb{E}_Z[q_h^2(X - Z)]} + 2||q||_\infty h^{-d}\varepsilon/3 \right)$$

We get ..... □

10.5 Universal Consistency

In the previous discussion, we have required the following conditions on the weights:

- $\int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^n \hat{w}_i(x) d(X_i, x)^2\right] dP(x) \to 0$ when n tends to infinity, to ensure that the bias goes to zero.
- $\int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^n \hat{w}_i(x)^2\right] dP(x) \to 0$ when n tends to infinity, to ensure that the variance goes to zero.

These were enough to show consistency when the target function is Lipschitz-continuous in $\mathbb{R}^d$ as seen in Eq.(10.6). These also led to a precise rate of convergence (which turned out to be optimal).

In order to show universal consistency for any square-intergrable functions, we need an extra (technical) assumption, which was first outlined in Stone's theorem, namely that there exists $c > 0$ such that for any non-negative integrable function $h : \mathcal{X} \mapsto \mathbb{R}$,

$$\int_{\mathcal{X}} \sum_{i=1}^{n} \mathbb{E}_{S_n}\left[\hat{w}_i(x) h(X_i)\right] dP(x) \leq c \cdot \int_{\mathcal{X}} h(x) dP(x) \tag{10.11}$$

Again, we only take the expectation with respect to the training data, while we use the integral notation to take the expectation with respect to the training distribution P.

In the following contents, h will be the **squared deviation (distance) between two functions**. Then for any $\varepsilon > 0$, and for any $f^* \in L_2(P(x))$, we can find a function g which is $B(\varepsilon)$-Lipschitz-continuous and such that $||f^* - g||_{L_2(P(x))} \leq \varepsilon$, that is because the set of Lipschitz-continuous functions is dense in $L_2(P(x))$

(Ambrosio, Gigli, and Savaré 2013). Then for a given $X \in \mathcal{X}$, we have

$$\begin{aligned}
&\mathbb{E}_{S_n}\left(\sum_{i=1}^{n} \hat{w}_i(x)[f^*(X_i) - f^*(X)]\right)^2 \\
&\leq \mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\Big[\big|f^*(X_i) - g(X_i)\big| + \big|g(X_i) - g(x)\big| + \big|g(x) - f^*(X)\big|\Big]\right)^2 \\
&\leq 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\big|f^*(X_i) - g(X_i)\big|\right)^2 + 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\big|g(X_i) - g(x)\big|\right)^2 + 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\big|g(x) - f^*(x)\big|\right)^2 \quad (1) \\
&\leq 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\big|f^*(X_i) - g(X_i)\big|\right)^2 + 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)B(\varepsilon)d(X_i, x)\right)^2 + 3\mathbb{E}\big|g(x) - f^*(x)\big|^2 \quad (2) \\
&\leq 3\mathbb{E}\left(\sum_{i=1}^{n} \hat{w}_i(x)\big|f^*(X_i) - g(X_i)\big|\right)^2 + 3B(\varepsilon)^2 \cdot \mathbb{E}\left[\sum_{i=1}^{n} \hat{w}_i(x)d(X_i, x)^2\right] + 3\mathbb{E}\big|g(x) - f^*(x)\big|^2 \quad (3) \\
&\leq 3c \cdot \mathbb{E}\big|f^*(x) - g(x)\big|^2 + 3B(\varepsilon)^2 \cdot \mathbb{E}\left[\sum_{i=1}^{n} \hat{w}_i(x)d(X_i, x)^2\right] + 3\mathbb{E}\big|g(x) - f^*(x)\big|^2
\end{aligned}$$

The inequality (1) is obtained using that $(a+b+c)^2 \leq 3a^2 + 3b^2 + 3c^2$, inequality (2) is due to the fact that weights summing to one and function g is Lipschitz-continuous, while inequality (3) applys the Jensen's inequality to the second term and the last inequality is a direct result of Eq.(10.11). We can now integrate with respect to $X = x$ and utilize the assumption that $||f^* - g||_{L_2(P(x))} \leq \varepsilon$ to get

$$\int_{\mathcal{X}} \mathbb{E}_{S_n}\left(\sum_{i=1}^{n} \hat{w}_i(x)[f^*(X_i) - f^*(x)]\right)^2 dP(x) \leq 3(c+1)\varepsilon^2 + 3B(\varepsilon)^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)d(X_i, x)^2\right] dP(x)$$

Proving universal consistency. We can then substitue the upper-bound of bias term into the first inequality of Eq.(10.5), which is

$$\begin{aligned}
\int_{\mathcal{X}} \mathbb{E}_{S_n}(\hat{f}(x) - f^*(x))^2 dP(x) &\leq \int_{\mathcal{X}} \mathbb{E}_{S_n}\left(\sum_{i=1}^{n} \hat{w}_i(x) \cdot \Big|f^*(X_i) - f^*(X)\Big|\right)^2 dP(x) + \sigma^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)^2\right] dP(x) \\
&\leq 3(c+1)\varepsilon^2 + 3B(\varepsilon)^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)d(X_i, x)^2\right] dP(x) + \sigma^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)^2\right] dP(x)
\end{aligned} \quad (10.12)$$

which is similar to the bound in Eq.(10.6). Next we can use the same tools for consistency as for Eq.(10.6).

In order to prove universal consistency, we fix a certain ε, from which we obtain some $B(\varepsilon)$. For such a $B(\varepsilon)$, we know how to obtain an overall term

$$3B(\varepsilon)^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)d(X_i, x)^2\right] dP(x) + \sigma^2 \int_{\mathcal{X}} \mathbb{E}_{S_n}\left[\sum_{i=1}^{n} \hat{w}_i(x)^2\right] dP(x)$$

for a well chosen hyperparameter and number of observations n as previous section. Thus, if the extra condition in Eq.(10.11) is satisfied, these three methods are universally consistent. We can now look at the cases

- Partitioning: Let $c = 2$ in Eq.(10.11) and we get universal consistency. This is because

$$\begin{aligned}
\sum_{i=1}^{n} \mathbb{E}_{S_n}[\hat{w}_i(x) f(X_i)] &= \sum_{j \in J} \sum_{i=1}^{n} \mathbb{E}_{S_n}\left[\hat{w}_i(x) \mathbb{1}_{x \in A_j} f(X_i)\right] \\
&= \sum_{j \in J} \mathbb{E}_{S_n}\left[\mathbb{1}_{x \in A_j}\left(\mathbb{1}_{n_{A_j} > 0} \cdot \frac{1}{n_{A_j}} \sum_{i \in A_j} f(X_i) + \mathbb{1}_{n_{A_j} = 0} \cdot \frac{1}{n} \sum_{i=1}^{n} f(X_i)\right)\right] \\
&\leq \sum_{j \in J} \mathbb{E}_{S_n}\left[\mathbb{1}_{x \in A_j}\left(\mathbb{E}[f(Z) \mid Z \in A_j] + \frac{1}{n} \sum_{i=1}^{n} f(X_i)\right)\right] \quad (X_i, i = 1, \ldots, n \text{ i.i.d}) \\
&= 2 \sum_{j \in J} \mathbb{1}_{x \in A_j} \mathbb{E}_{S_n}[f(X)] = 2\mathbb{E}_{S_n}[f(X)]
\end{aligned}$$

- Kernel regression: it can be shown using the same type of techiniques outlined for oonsistency for Lipschitz-continuous functions

- k-nearest neighbor: the condition in Eq.(10.11) is not easy to show, and is often referred to as Stone's lemma.

11 Sparse Methods

12 Neural Networks

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Appendices

A Norms

A.1 Norms

A function $f : \mathbb{R}^n \to \mathbb{R}$ with dom $f = \mathbb{R}^n$ is called a norm if

- f is nonnegative: $f(x) \geq 0$ for all $x \in \mathbb{R}$
- f is definite: $f(x) = 0$ only if $x = 0$
- f is homogeneous: $f(tx) = |t|f(x)$, for all $x \in \mathbb{R}^n$ and $t \in \mathbb{R}$
- f satisfies the triangle inequality: $f(x + y) \leq f(x) + f(y)$, for all $x, y \in \mathbb{R}^n$

A norm is a measure of the length of a vector x; we can measure the distance between two vectors x and y as the length of their difference, *i.e.*

$$\mathrm{dist(x, y) = ||x - y||}$$

The set of all vectros with norm less than or equal to one,

$$\mathcal{B} = \{x \in \mathbb{R}^n \mid ||x|| \leq 1\}$$

is called the unit ball of the norm $|| \cdot ||$. The unit ball satisfies the following properties:

- $\mathcal{B}$ is symmetric about the origin; $x \in \mathcal{B}$ iff $-x \in \mathcal{B}$
- $\mathcal{B}$ is convex
- $\mathcal{B}$ is closed, bounded, and has nonempty interior

A.2 Examples of Norm

Here we consider the norm for vector $x \in \mathbb{R}^n$

- l_1-norm
$$||x||_1 = |x_1| + \cdots + |x_n|$$
- l_∞-norm
$$||x||_\infty = \max\{|x_1|, \ldots, |x_n|\}$$
- l_p-norm
$$||x||_p = \left(|x_1|^p + \cdots + |x_n|^p\right)^{1/p}$$
- P-quadratic norms: for matrix $P \in \mathbb{S}^n_{++}$,
$$||x||_P = (x^\top Px)^{1/2} = ||P^{1/2}x||_2$$

  The unit ball of a quadratic norm is an ellipsoid (and conversely, if the unit ball of a norm is an ellipsoid, the norm is a quadratic norm)

- Frobenius norm: for matrix $X \in \mathbb{R}^{m \times n}$,

$$||X||_F = \left(\mathrm{tr}(\mathrm{X}^\top \mathrm{X})\right)^{1/2} = \left(\sum_{\mathrm{i=1}}^{\mathrm{m}} \sum_{\mathrm{j=1}}^{\mathrm{n}} \mathrm{X}_{\mathrm{ij}}^2\right)^{1/2} \tag{A.1}$$

  The Frobenius norm is the Euclidean norm of the vector obtained by listing the coefficients of the matrix. It is different from the l_2-norm of matrix.

A.3 Equivalence of Norms

Suppose that $||\cdot||_a$ and $||\cdot||_b$ are norms on $\mathbb{R}^n$. A basic result of analysis is that there exist positive constants α and β such that, for all $x \in \mathbb{R}$,

$$\alpha||x||_a \leq ||x||_b \leq \beta||x||_a$$

This means that the norms are equivalent, i.e., they define the same set of open subsets, the same set of covergent sequences, and so on. Using convex analysis, we can give a more specific result: if $||\cdot||$ is any norm on $\mathbb{R}^n$, then there exists a quadratic norm $||\cdot||_P$ for which

$$||x||_P \leq ||x|| \leq \sqrt{n}||x||_P$$

holds for all x. In other words, any norm on $\mathbb{R}^n$ can be uniformly approximated, within a factor of $\sqrt{n}$, by a P-quadratic norm. *We conclude that any norms on all finite-dimensional vector space are equivalent, but on infinite-dimensional vector spaces, the result need not hold.*

Theorem A.1 (Holder's Inequality)**.** Let (S, σ, μ) be a measure space and let $p, q \in [1, \infty]$ with $1/p + 1/q = 1$. Then for all measurable real- or complex-valued functions f and g on S,

$$||fg||_1 \leq ||f||_p ||g||_q \tag{A.2}$$

If, in addition, $p, q \in (1, \infty)$ and $f \in L_p(\mu)$ and $g \in L_q(\mu)$, then Holder's inequality becomes an equality if and only if $|f|_p$ and $|g|_q$ are linearly dependent in $L_1(\mu)$, meaning that there exist real numbers $\alpha, \beta \geq 0$, not both of them zero, such that $\alpha|f|_p = \beta|g|_q$ μ-almost everywhere.

The pair of numbers (p, q) are called conjugate pair and the special case of $p = q = 2$ gives a form of the Cauchy-Schwarz inequality.

A.4 Operator Norms

Supose $||\cdot||_a$ and $||\cdot||_b$ are norms on $\mathbb{R}^m$ and $\mathbb{R}^n$, respectively. We define the *opertaor norm* of $X \in \mathbb{R}^{m \times n}$, induced by the norms $||\cdot||_a and ||\cdot||_b$, as

$$||X||_{a,b} = \sup\left\{||Xu||_a \mid ||u||_b \leq 1\right\} \tag{A.3}$$

It can be shown that this defines a norm on $\mathbb{R}^{m \times n}$.

- When $||\cdot||_a$ and $||\cdot||_b$ are both Euclidean norms, the operator norm of X is its *maximum singular value*, and is denoted $||X||_2$:

$$||X||_2 = \sigma_{\max}(X) = \left(\lambda_{\max}(X^\top X)\right)^{1/2} \tag{A.4}$$

That is because, $X^\top X$ is a symmetric matrix, which satisfy

$$u^\top (X^\top X)u \leq \lambda_{\max}(X^\top X)u^\top u$$

This agress with the Euclidean norm on $\mathbb{R}^m$, when $X \in \mathbb{R}^{m\times 1}$, so there is not clash of notation. This norm is also called the *spectral norm* or l_2*-norm* of X.

- The norm induced by the l_∞-norm on $\mathbb{R}^m$ and $\mathbb{R}^n$, denoted $||X||_\infty$, is the *max-row-sum* norm

$$||X||_\infty = \sup\left\{||Xu||_\infty \mid ||u||_\infty \leq 1\right\} = \max_{i=1,\ldots,m} \sum_{j=1}^{n} |X_{ij}|$$

- The norm induced by the l_1-norm on $\mathbb{R}^m$ and $\mathbb{R}^n$, denoted $||X||_1$, is the *max-column-sum* norm

$$||X||_1 = \max_{j=1,\ldots,n} \sum_{i=1}^{m} |X_{ij}|$$

B Probability Theory

B.1 Independence

Definition B.1 (Independent)**.** Two random variables X and Y are independent if, for every A and B,

$$\mathbb{P}(X \in A, Y \in B) = \mathbb{P}(X \in A)\mathbb{P}(Y \in B)$$

and we write $X \perp\!\!\!\perp Y$.

In principle, to check whether X and Y are independent we need to check the above equation for all subsets A and B. Fortunately, we have the following result which we state for continuous random variables though it is true for discrete random variables too.

Theorem B.1. Let X and Y have joint PDF $f_{X,Y}$. Then $X \perp\!\!\!\perp Y$ if and only if

$$f_{X,Y}(x, y) = f_X(x)f_Y(y)$$

for all values x and y.

Definition B.2 (Conditional Independent)**.** Let X, Y and Z be random variables. X and Y are conditionally independent given Z, wirtten $X \perp\!\!\!\perp Y \mid Z$, if

$$f_{X,Y|Z}(x, y \mid z) = f_{X|Z}(x \mid z)f_{Y|Z}(y \mid z)$$

for all x, y and z.

Intuitively, this means that, once you know Z, Y provides no extra information about X. An equivalent definition is that

$$f_{X|Y,Z}(x \mid y, z) = f_{X|Z}(x \mid z)$$

Here are some rules of the conditional independence:

- **Symmetry**

$$X \perp\!\!\!\perp Y \quad \Rightarrow \quad Y \perp\!\!\!\perp X$$

- **Decomposition**

$$X \perp\!\!\!\perp (A,B) \quad \Rightarrow \quad \text{and} \begin{cases} X \perp\!\!\!\perp A \\ X \perp\!\!\!\perp B \end{cases}$$

  Proof:

$$\begin{aligned} f_{X,A}(x,a) &= \int_B f_{X,A,B}(x,a,b)db \\ &= \int_B f_X(x) f_{A,B}(a,b)db \\ &= f_X(x) f_A(a) \end{aligned}$$

  A similar proof shows the independence of X and B.

- **Weak Union**

$$X \perp\!\!\!\perp (A,B) \quad \Rightarrow \quad \text{and} \begin{cases} X \perp\!\!\!\perp A \mid B \\ X \perp\!\!\!\perp B \mid A \end{cases}$$

  Proof:

  - by assumption, we have $\mathbb{P}(X) = \mathbb{P}(X \mid A, B)$
  - due to the property of decomposition $X \perp\!\!\!\perp B$, we have $\mathbb{P}(X) = \mathbb{P}(X \mid B)$

  Combining the above two equalities yields

$$\mathbb{P}(X \mid B) = \mathbb{P}(X \mid A, B)$$

  which establishes $X \perp\!\!\!\perp A \mid B$. A similar proof shows the second condition.

- **Contraction**

$$\left.\begin{aligned} X \perp\!\!\!\perp A \mid B \\ X \perp\!\!\!\perp B \end{aligned}\right\} \text{ and } \quad \Rightarrow \quad X \perp\!\!\!\perp (A,B)$$

  or similarily

$$\left.\begin{aligned} X \perp\!\!\!\perp B \mid A \\ X \perp\!\!\!\perp A \end{aligned}\right\} \text{ and } \quad \Rightarrow \quad X \perp\!\!\!\perp (A,B)$$

  Proof: this property can be proved by noticing that

$$\mathbb{P}(X \mid A, B) = \mathbb{P}(X \mid B) = \mathbb{P}(X)$$

  each equality of which is asserted by $X \perp\!\!\!\perp A \mid B$ and $X \perp\!\!\!\perp B$, respectively. A similar proof shows the second one.

- **Intersection**

  for strictly positive probability distributions, the following also hold

$$\left.\begin{aligned} X \perp\!\!\!\perp Y \mid Z, W \\ X \perp\!\!\!\perp W \mid Z, Y \end{aligned}\right\} \text{ and } \quad \Rightarrow \quad X \perp\!\!\!\perp (W,Y) \mid Z$$

  Proof: by assumption

$$\mathbb{P}(X \mid Z, W, Y) = \mathbb{P}(X \mid Z, W) = \mathbb{P}(X \mid Z, Y)$$

Using this equality, together with the law of total probability applied to $\mathbb{P}(X \mid Z)$

$$\begin{aligned}\mathbb{P}(X \mid Z) &= \sum_{w \in W} \mathbb{P}(X \mid Z, W = w)\mathbb{P}(W = w \mid Z)\\ &= \sum_{w \in W} \mathbb{P}(X \mid Y, Z)\mathbb{P}(W = w \mid Z)\\ &= \mathbb{P}(X \mid Z, Y) \sum_{w \in W} \mathbb{P}(W = w \mid Z)\\ &= \mathbb{P}(X \mid Z, Y)\end{aligned}$$

This suggest

$$\mathbb{P}(X \mid Z, W, Y) = \mathbb{P}(X \mid Z)$$

which establishs $X \perp\!\!\!\perp (W, Y) \mid Z$.

In general, we have

$$\begin{aligned} X \perp\!\!\!\perp (Y, Z) \quad &\Leftrightarrow \quad X \perp\!\!\!\perp Y \text{ and } X \perp\!\!\!\perp Y \mid Z\\ &\Leftrightarrow \quad X \perp\!\!\!\perp Z \text{ and } X \perp\!\!\!\perp Z \mid Y \end{aligned} \tag{B.1}$$

B.2 Expectations

Definition B.3. The expectation, or mean, or first moment, of random variable X is defined to be

$$\mathbb{E}[X] = \int_{\mathcal{X}} x dF(x) = \begin{cases} \sum_{\mathcal{X}} x f(x) \\ \int_{\mathcal{X}} x f(x) dx \end{cases}$$

assuming that the sum (or integral) is well defined.

Theorem B.2. Let $Y = r(X)$, then

$$\mathbb{E}[Y] = \mathbb{E}[r(X)] = \int_{\mathcal{X}} r(x) dF_X(x)$$

Definition B.4. The conditional expectation of X given $Y = y$ is

$$\mathbb{E}[X \mid Y = y] = \int_{-\infty}^{\infty} x f_{X|Y}(x) dx$$

If $r(x, y)$ is a function of x and y then

$$\mathbb{E}[r(X, Y) \mid Y = y] = \int_{-\infty}^{\infty} r(x, y) f_{X|Y}(x) dx$$

Theorem B.3 (Law of Total Expectations)**.** For random variables X and Y, assumping $\mathbb{E}[X]$ and $\mathbb{E}[Y]$ exists, then we have

$$\mathbb{E}\big[\mathbb{E}[X \mid Y]\big] = \mathbb{E}[X]$$

and more generally for any function $r(x, y)$

$$\mathbb{E}\big[\mathbb{E}[r(X, Y) \mid X]\big] = \mathbb{E}[r(X, Y)]$$

Proof. By definition B.4, we have

$$\begin{aligned}
\mathbb{E}\big[\mathbb{E}[X \mid Y]\big] &= \int_{-\infty}^{\infty} \mathbb{E}[X \mid Y = y] f_Y(y) dy \\
&= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} x f_{X|Y}(x) dx \right) f_Y(y) dy \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x \frac{f_{X,Y}(x, y)}{f_Y(y)} f_Y(y) dx dy \\
&= \int_{-\infty}^{\infty} x dx \int_{-\infty}^{\infty} f_{X,Y}(x, y) dy \\
&= \int_{-\infty}^{\infty} x f_X(x) dx = \mathbb{E}[X]
\end{aligned}$$

and similarily, we have

$$\begin{aligned}
\mathbb{E}\big[\mathbb{E}[r(X, Y) \mid Y]\big] &= \int_{-\infty}^{\infty} \mathbb{E}[r(X, Y) \mid Y = y] f_Y(y) dy \\
&= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} r(x, y) f_{X|Y}(x) dx \right) f_Y(y) dy \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} r(x, y) f_{X,Y}(x, y) dx dy \\
&= \mathbb{E}[r(X, Y)]
\end{aligned} \tag{B.2}$$

□

Corollary B.4 (Law of Iterated Expectation)**.** For random variables X, Y, Z, we have

$$\mathbb{E}\big[\mathbb{E}[Z \mid X, Y] \mid Y\big] = \mathbb{E}[Z \mid Y] = \mathbb{E}\big[\mathbb{E}[Z \mid Y] \mid X, Y\big]$$

Proof. The first equality holds because of the fact that, for any y

$$\begin{aligned}
\mathbb{E}\big[\mathbb{E}[Z \mid X, Y] \mid Y = y\big] &= \mathbb{E}[r(X, Y) \mid Y = y] \\
&= \int_{-\infty}^{\infty} r(X, Y) f_{X|Y}(x) dx \\
&= \int_{-\infty}^{\infty} \mathbb{E}[Z \mid X, Y] f_{X|Y}(x) dx \\
&= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} z f_{Z|X,Y}(z) dz \right) f_{X|Y}(x) dx \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} z \frac{f_{Z,X,Y}(z, x, y)}{f_{X,Y}(x, y)} \frac{f_{X,Y}(x, y)}{f_Y(y)} dx dz \\
&= \int_{-\infty}^{\infty} z dz \int_{-\infty}^{\infty} f_{Z,X|Y}(z, x) dx \\
&= \int_{-\infty}^{\infty} z f_{Z|Y}(z) dz = \mathbb{E}[Z \mid Y = y]
\end{aligned}$$

and for any y

$$\begin{aligned}\mathbb{E}\big[\mathbb{E}[X \mid Y] \mid X, Y = y\big] &= \mathbb{E}\big[\mathbb{E}[X \mid Y = y] \mid X, Y = y\big] \\ &= \mathbb{E}[X \mid Y = y] \cdot \mathbb{E}[1 \mid X, Y = y] = \mathbb{E}[X \mid Y = y]\end{aligned}$$

□

Theorem B.5 (Independencec)**.** For random variables X and Y, we have

$$\mathbb{E}[XY] = \mathbb{E}[X \mid Y] \cdot \mathbb{E}[Y]$$

If X is independent of Y, i.e. $X \perp\!\!\!\perp Y$, then we have

$$\mathbb{E}[X \mid Y] = \mathbb{E}[X]$$

and consequently

$$\mathbb{E}[XY] = \mathbb{E}[X] \cdot \mathbb{E}[Y]$$

Proof. By definition

$$\begin{aligned}\mathbb{E}[X \mid Y] &= \int x f_{X|Y}(x) dx \\ &= \int x \frac{f_{X,Y}(x,y)}{f_Y(y)} dx \\ &= \int x f_X(x) dx \qquad (X \perp\!\!\!\perp Y) \\ &= \mathbb{E}[X]\end{aligned}$$

□

Definition B.5. The condtional variance is defined as

$$\begin{aligned}\operatorname{Var}(X \mid Y = y) &= \mathbb{E}\big(X - \mathbb{E}[X \mid Y = y]\big)^2 \\ &= \int_{-\infty}^{\infty} \big(x - \mathbb{E}[X \mid Y = y]\big)^2 f_{X|Y}(x) dx\end{aligned} \tag{B.3}$$

Theorem B.6 (Law of Total Variance)**.** For random variables X and Y,

$$\operatorname{Var}(X) = \mathbb{E}[\operatorname{Var}(X \mid Y)] + \operatorname{Var}(\mathbb{E}[X \mid Y]) \tag{B.4}$$

Proof. Notice that

$$\begin{aligned}\mathbb{E}[\operatorname{Var}(X \mid Y)] &= \mathbb{E}\Big[\mathbb{E}[X^2 \mid Y] - \mathbb{E}[X \mid Y]^2\Big] \\ &= \mathbb{E}[X^2] - \mathbb{E}\big[\mathbb{E}[X \mid Y]^2\big]\end{aligned}$$

and

$$\begin{aligned}\operatorname{Var}(\mathbb{E}[X \mid Y]) &= \mathbb{E}\big[\mathbb{E}[X \mid Y]^2\big] - \mathbb{E}\big[\mathbb{E}[X \mid Y]\big]^2 \\ &= \mathbb{E}\big[\mathbb{E}[X \mid Y]^2\big] - \mathbb{E}[X]^2\end{aligned}$$

Adding these two together yields $\operatorname{Var}(X)$. □

Corollary B.7 (Law of Total Covariance)**.** For random variable X, Y and Z,

$$\operatorname{Cov}(X, Y) = \mathbb{E}\big[\operatorname{Cov}(X, Y \mid Z)\big] + \operatorname{Cov}\big(\mathbb{E}[X \mid Z], \mathbb{E}[Y \mid Z]\big) \tag{B.5}$$

B.3 Convergences

Definition B.6 (Type of Convergence)**.** Let $X_1, X_2, \dots,$ be a sequence of random variables and let X be another random variable. Let F_n denote the CDF of X_n and let F denote the CDF of X_n and F the CDF of X.

1. X_n converges to X **in quadratic mean** (convergence in L_2), written $X_n \xrightarrow{qm} X$, if
$$\mathbb{E}[X_n - X]^2 \to 0 \tag{B.6}$$
as $n \to \infty$.
2. X_n converges to x in L_1, written $X_n \xrightarrow{L_1} X$, if
$$\mathbb{E}|X_n - X| \to 0 \tag{B.7}$$
as $n \to \infty$.
3. X_n converges to X **almost surely**, written $X_n \xrightarrow{a.s.} X$, if
$$\mathbb{P}\big(\{s : X_n(s) \to X(s)\}\big) = 1 \tag{B.8}$$
4. X_n converges to X **in probability**, written $X_n \xrightarrow{P} X$, if, for every $\varepsilon > 0$,
$$\mathbb{P}(|X_n - X| > \varepsilon) \to 0 \tag{B.9}$$
as $n \to \infty$.
5. X_n converges to X **in distribution**, written $X_n \rightsquigarrow X$, if
$$\lim_{n\to\infty} F_n(t) = F(t) \tag{B.10}$$
at all t for which F is continuous

Theorem B.8. The following relationships hold:

1. $X_n \xrightarrow{qm} X$ implies that $X_n \xrightarrow{L_1} X$
2. $X_n \xrightarrow{L_1} X$ implies that $X_n \xrightarrow{P} X$
3. $X_n \xrightarrow{a.s.} X$ implies that $X_n \xrightarrow{P} X$
4. $X_n \xrightarrow{qm} X$ implies that $X_n \xrightarrow{P} X$
5. $X_n \xrightarrow{P} X$ implies that $X_n \rightsquigarrow X$
6. If $X_n \rightsquigarrow X$ and if $\mathbb{P}(X = c) = 1$ for some real number c, then $X_n \xrightarrow{P} P$

In general, none of the reverse implications hold except the special case in 3.

Proof. Consider the following

1. Suppose

2.

3.

4. Suppose that $X_n \xrightarrow{qm} X$. Fix $\varepsilon > 0$ and use Markov's inequalit,

$$\mathbb{P}(|X_n - X| > \varepsilon) = \mathbb{P}(|X_n - X|^2 > \varepsilon^2) \leq \frac{\mathbb{E}|X_n - X|^2}{\varepsilon^2} \to 0$$

5. Fix $\varepsilon > 0$ and let x be a continuity point of F, then

$$\begin{aligned} F_n(x) = \mathbb{P}(X_n \leq x) &= \mathbb{P}(X_n \leq x, X \leq x + \varepsilon) + \mathbb{P}(X_n \leq x, X > x + \varepsilon) \\ &\leq \mathbb{P}(X \leq x + \varepsilon) + \mathbb{P}(|X_n - X| > \varepsilon) \\ &= F(x + \varepsilon) + \mathbb{P}(|X_n - X| > \varepsilon) \end{aligned}$$

Also,

$$\begin{aligned} F(x - \varepsilon) = \mathbb{P}(X \leq x - \varepsilon) &= \mathbb{P}(X \leq x - \varepsilon, X_n \leq x) + \mathbb{P}(X \leq x - \varepsilon, X_n > x) \\ &\leq F_n(x) + \mathbb{P}(|X_n - X| > \varepsilon) \end{aligned}$$

Hence,

$$F(x - \varepsilon) - \mathbb{P}(|X_n - X| > \varepsilon) \leq F_n(x) \leq F(x + \varepsilon) + \mathbb{P}(|X_n - X| > \varepsilon)$$

Take the limit as $n \to \infty$ to conclude that

$$F(x - \varepsilon) \leq \lim_{n \to \infty} \inf F_n(x) \leq \lim_{n \to \infty} \sup F_n(x) \leq F(x + \varepsilon)$$

This holds for any $\varepsilon > 0$. Take the limit as $\varepsilon \to 0$ and use the fact that F is continuous at x, we conclude that

$$\lim_{n \to \infty} F_n(x) = F(x)$$

6. Fix $\varepsilon > 0$, then

$$\begin{aligned} \mathbb{P}(|X_n - c| > \varepsilon) &= \mathbb{P}(X_n < c - \varepsilon) + \mathbb{P}(X_n > c + \varepsilon) \\ &\leq \mathbb{P}(X_n \leq c - \varepsilon) + \mathbb{P}(X_n > c + \varepsilon) \\ &= F_n(c - \varepsilon) + 1 - F_n(c + \varepsilon) \\ &\to F(c - \varepsilon) + 1 - F(c + \varepsilon) \\ = 0 + 1 - 1 = 0 \end{aligned}$$

□

Theorem B.9 (Slutsky's Theorem)**.** Let X_n, Y_n and X, Y be random variables,

1. If $X_n \xrightarrow{P} X$ and $Y_n \xrightarrow{P} Y$, then $X_n + Y_n \xrightarrow{P} X + Y$
2. If $X_n \xrightarrow{P} X$ and $Y_n \xrightarrow{P} Y$, then $X_n Y_n \xrightarrow{P} XY$
3. If $X_n \rightsquigarrow X$ and $Y_n \rightsquigarrow c$, then $X_n + Y_n \rightsquigarrow X + c$
4. If $X_n \rightsquigarrow X$ and $Y_n \rightsquigarrow c$, then $X_n Y_n \rightsquigarrow cX$

Theorem B.10 (Continuous Mapping Theorem)**.** Let X be a random variable, X_n be a sequence of random variables and g be a continuous function.

1. If $X_n \xrightarrow{a.s.} X$, then $g(X_n) \xrightarrow{a.s.} g(X)$
2. If $X_n \xrightarrow{P} X$, then $g(X_n) \xrightarrow{P} g(X)$
3. If $X_n \rightsquigarrow X$, then $g(X_n) \rightsquigarrow g(X)$

Theorem B.11 (The Weak Law of Large Numbers)**.** If $X_1, \dots, X_n$ are I.I.D, then

$$\bar{X}_n \xrightarrow{P} \mu$$

WLLN means that the distribution of $\bar{X}_n$ becomes more concentrated around μ as n gets large.

Proof. Assume that $\sigma < \infty$. This is not necessary but it simplifies the proof. Using Chebyshev inequality,

$$\mathbb{P}(|\bar{X}_n - \mu| \geq \varepsilon) \leq \frac{\operatorname{Var}(\bar{X}_n)}{\varepsilon^2} = \frac{\sigma^2}{n\varepsilon^2} \to 0$$

□

Theorem B.12 (The Central Limit Theorem)**.** Let $X_1, \dots, X_n$ be I.I.D with mean μ and variance σ^2, then

$$Z_n \equiv \frac{\bar{X}_n - \mu}{\sqrt{\operatorname{Var}(\bar{X}_n)}} = \frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma} \rightsquigarrow Z \tag{B.11}$$

where $Z \sim N(0,1)$. In other words,

$$\lim_{n\to\infty} \mathbb{P}(Z_n \leq z) = \Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx \tag{B.12}$$

CLT suggests that the distribution (CDF, not PDF) of $\bar{X}_n$ can be approximated using a Normal disitribution. It's the probability statements that we are approximating, not the random variable itself.

Proof. Suppose there are n I.I.D random variables X_i with mean μ and variance σ^2. Let

$$Y_i = \frac{X_i - \mu}{\sigma}$$

and

$$Z_n = \frac{\sum_i Y_i}{\sqrt{n}} = \frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma}$$

Suppose the moment generating function (MGF) of Y_i is $\varphi_Y(t) = \mathbb{E}[e^{tY}]$, and it is finite in a neighborhood around $t = 0$. Then we have

$$\varphi_{Y_1+\cdots+Y_n}(t) = \mathbb{E}\left[e^{t(Y_1+\cdots+Y_n)}\right] = \mathbb{E}\left[e^{tY_i}\right]^n = \left(\varphi_Y(t)\right)^n$$

and consequently

$$\varphi_{Z_n}(t) = \mathbb{E}\left[e^{t\frac{Y_1+\cdots+Y_n}{\sqrt{n}}}\right] = \left[\varphi_Y\left(\frac{t}{\sqrt{n}}\right)\right]^n$$

Notice that

$$\varphi_Y'(0) = \mathbb{E}[Y] = 0 \quad \text{and} \quad \varphi_Y''(0) = \mathbb{E}[Y^2] = \operatorname{Var} Y = 1$$

So the Taylor expansion gives us

$$\begin{aligned}\varphi_Y(t) &= \varphi_Y(0) + t\varphi_Y'(0) + \frac{t^2}{2!}\varphi_Y''(0) + \frac{t^3}{3!}\varphi_Y'''(0) + \cdots \\ &= 1 + 0 + \frac{t^2}{2} + \frac{t^3}{3!}\varphi_Y'''(0) + \cdots \\ &= 1 + \frac{t^2}{2} + \frac{t^3}{3!}\varphi_Y'''(0) + \cdots\end{aligned}$$

Therefore,

$$\begin{aligned}\varphi_{Z_n}(t) &= \left[\varphi_Y\left(\frac{t}{\sqrt{n}}\right)\right]^n \\ &= \left[1 + \frac{t^2}{2!n} + \frac{t^3}{3!n^{3/2}}\varphi_Y'''(0) + \cdots\right]^n \\ &= \left[1 + \frac{\frac{t^2}{2} + \frac{t^3}{3!n^{1/2}}\varphi'''(0) + \cdots}{n}\right]^n \\ &\to e^{t^2/2}\end{aligned}$$

The last step results from the fact that $\left(1 + \frac{a_n}{n}\right)^n \to e^a$ if $a_n \to a$. Notice that the MGF of standard normal variable $Z \sim N(0,1)$ is just

$$\varphi_Z(t) = \mathbb{E}\left[e^{tZ}\right] = e^{t^2/2}$$

So we have

$$\varphi_{Z_n}(t) \to \varphi_Z(t) \quad \Rightarrow \quad Z_n \rightsquigarrow Z$$

□

Example. CLT implies that $Z_n = \sqrt{n}(\bar{X}_n - \mu)/\sigma$ approximately follows $N(0,1)$. However, we rarely know σ. Instead, we can estimate σ^2 from i.i.d samples $X_1, \ldots, X_n$ by

$$S_n^2 = \frac{1}{n-1}\sum_{i=1}^n (X_i - \bar{X}_n)^2$$

Suppose the assumptions in CLT hold, prove the following

- $S_n^2 \xrightarrow{P} \sigma^2$
- $\sqrt{n}(\bar{X}_n - \mu)/S_n \rightsquigarrow N(0,1)$

Proof. For the first statement, notice that by CLT, we have

$$\frac{1}{n}\sum_{i=1}^n X_i \xrightarrow{P} \mathbb{E}[X]$$

$$\frac{1}{n}\sum_{i=1}^n X_i^2 \xrightarrow{P} \mathbb{E}[X^2]$$

Therefore, we can utilize the continuous mapping theorem (or Slutsky's theorem) and get

$$\begin{aligned} S_n^2 &= \frac{n}{n-1}\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2 \\ &= \frac{n}{n-1}\left(\frac{1}{n}\sum_{i=1}^{n}X_i^2 - \left(\frac{1}{n}\sum_{i=1}^{n}X_i\right)^2\right) \\ &= \frac{n}{n-1}\left(\mathbb{E}[X^2] - \mathbb{E}[X]^2\right) \quad \text{(continous mapping theorem)} \\ &= \frac{n}{n-1}\sigma^2 \to \sigma^2 \quad (\text{as } n \to \infty) \end{aligned}$$

Now, the second statement can be shown trivially by Slutsky's theorem, that is

$$\frac{\sqrt{n}(\bar{X}_n - \mu)}{S_n} = \frac{\sqrt{n}(\bar{X}_n - \mu)}{\sigma}\frac{\sigma}{S_n} \rightsquigarrow N(0,1)$$

by noticing that $\frac{\sqrt{n}(\bar{X}_n-\mu)}{\sigma} \rightsquigarrow N(0,1)$ and $\sigma/S_n \xrightarrow{P} 1$. □

Theorem B.13 (Multivariate Central Limit Theorem)**.** Let $X_1, \ldots, X_n$ be IID random vectors where

$$X_i = (X_{1i}\ X_{2i} \cdots X_{ki})^\top$$

with mean

$$\mu = (\mu_1\ \mu_2 \cdots \mu_k)^\top = (\mathbb{E}[X_{1i}]\ \mathbb{E}[X_{2i}] \cdots \mathbb{E}[X_{ki}])^\top$$

and variance matrix Σ. Let

$$\bar{X} = (\bar{X}_1\ \bar{X}_2 \cdots \bar{X}_k)$$

where $\bar{X}_j = n^{-1}\sum_{i=1}^n X_{ji}$. Then

$$\sqrt{n}(\bar{X} - \mu) \rightsquigarrow N(0, \Sigma)$$

If Y_n has a limiting Normal distribution then the delta method allows us to find the limiting distribution of $g(Y_n)$ where g is any smooth function (differentiable).

Theorem B.14 (The Delta Method)**.** Suppose that

$$\frac{\sqrt{n}(Y_n - \mu)}{\sigma} \rightsquigarrow N(0,1)$$

and that g is a differentiable function such that $g'(\mu) \neq 0$. Then

$$\frac{\sqrt{n}(g(Y_n) - g(\mu))}{|g'(\mu)|\sigma} \rightsquigarrow N(0,1)$$

In other words,

$$Y_n \simeq N\left(\mu, \frac{\sigma^2}{n}\right) \quad \text{implies that} \quad g(Y_n) \simeq N\left(g(\mu), (g'(\mu))^2\frac{\sigma^2}{n}\right) \tag{B.13}$$

Theorem B.15 (The Multivariate Delta Method)**.** Suppose that $Y_n = (Y_{n1}, \ldots, Y_{nk})$ is a sequence of random vectors such that

$$\sqrt{n}(Y_n - \mu) \rightsquigarrow N(0, \Sigma)$$

Let $g : \mathbb{R}^k \to \mathbb{R}$ and let

$$\nabla g(y) = \left(\frac{\partial g}{\partial y_1} \cdots \frac{\partial g}{\partial y_k} \right)^\top$$

Let ∇_μ denote $\nabla g(y)$ evaluated at $y = \mu$ and assume that the elements of ∇_μ are nonzero. Then

$$\sqrt{n}(g(Y_n) - g(\mu)) \rightsquigarrow N(0, \nabla_\mu^\top \Sigma \nabla_\mu)$$

C Concentration of Measure

C.1 Markov Inequality

Theorem C.1 (Markov Inequality)**.** For any nonnegative random variable $X \geq 0$

$$P(X \geq t) \leq \frac{\mathbb{E}[X]}{t} = O\left(\frac{1}{t}\right) \tag{C.1}$$

Proof.

$$\mathbb{E}[X] = \int_0^\infty xp(x)dx \geq \int_t^\infty xp(x)dx \geq t\int_t^\infty = t\mathbb{P}(X \geq t)$$

Similarily, we can apply the same calculation and get

$$\mathbb{E}\left[(X-\mu)^k\right] \geq t^k \mathbb{P}\left((X-\mu)^k \geq t^k\right) = t^k \mathbb{P}(|X-\mu| \geq t)$$

that is to say

$$\mathbb{P}(|X-\mu| \geq t) \leq \frac{\mathbb{E}\left[(X-\mu)^k\right]}{t^k} \tag{C.2}$$

□

C.2 Chebyshev Inequality

Theorem C.2 (Chebyshev Inequality)**.** For any random variable X with variance σ^2, for any $t \geq 0$

$$\mathbb{P}\big(|X-\mu| \geq t\sigma\big) \leq \frac{1}{t^2} \tag{C.3}$$

Proof. This could be obatained immediatly by choosing $k = 2$ and $t = n\sigma$ from inequality (C.2), that is,

$$\mathbb{P}\big(|X-\mu| \geq t\sigma\big) \leq \frac{\sigma^2}{t^2\sigma^2} = \frac{1}{t^2}$$

□

Here is an example. Consider the average of i.i.d. random variables with mean μ and variance σ^2

$$\bar{X}_n = \frac{1}{n}\sum_{i=1}^n X_i$$

It has mean μ and variance σ^2/n. Applying Chebyshev inequality, we have

$$\mathbb{P}\left(|\bar{X}_n - \mu| \geq \frac{t\sigma}{\sqrt{n}}\right) \leq \frac{1}{t^2}$$

with 0.99 proabability ($t = 10$), the average $\bar{X}_n$ would not exceed $\mu + 10\sigma/\sqrt{n}$. This would lead to the Weak Law of Large Numbers.

C.3 Chernoff's Methods

Theorem C.3 (Chernoff Bound)**.** Suppose the moment generating function of random variable X exists, and is finite for all $|t| \leq b, b > 0$. Let $\mu = \mathbb{E}[X]$, for any $t > 0$

$$\mathbb{P}((X - \mu) \geq u) \leq \inf_{0 \leq t \leq b} \frac{\mathbb{E}[e^{tX}]}{e^{(u+\mu)t}} \tag{C.4}$$

Proof. By Markov inequality, we have

$$\mathbb{P}((X - \mu) \geq u) = \mathbb{P}\left(e^{t(X-\mu)} \geq e^{tu}\right) \leq \frac{\mathbb{E}\left[e^{t(X-\mu)}\right]}{e^{tu}}$$

Since this bound is true for any t, we have

$$\mathbb{P}((X - \mu) \geq u) \leq \inf_{0 \leq t \leq b} \frac{\mathbb{E}[e^{tX}]}{e^{(u+\mu)t}}$$

□

Bounded Random Variables. We are going to consider the case of bounded random variables and derive the so called Hoeffding's bound for them. As we know, the bounded random variables are the special case of sub-Gaussian variables.

Lemma C.4 (MGF of Rademacher Variables)**.** The Rademacher variable is the random variable $X \in \{+1, -1\}$ with equally probability. The MGF of Rademacher variable satifies

$$\mathbb{E}[e^{tX}] \leq e^{t^2/2} \tag{C.5}$$

Proof. By definition,

$$\begin{aligned}\mathbb{E}[e^{tX}] = \frac{1}{2}(e^t + e^{-t}) &= \frac{1}{2}\left(\sum_{k=0}^{\infty} \frac{t^k}{k!} + \sum_{k=0}^{\infty} \frac{(-t)^k}{k!}\right) \\ &= \sum_{k=0}^{\infty} \frac{t^{2k}}{(2k)!} \leq \sum_{k=0}^{\infty} \frac{t^{2k}}{2^k k!} = e^{t^2/2}\end{aligned}$$

□

Lemma C.5 (Jensen's inequality)**.** A function g is convex if

$$g(\alpha x + (1 - \alpha)y) \leq \alpha g(x) + (1 - \alpha)g(y)$$

for all x, y and all $\alpha \in [0, 1]$; then for random variable X we have

$$g(\mathbb{E}[X]) \leq \mathbb{E}[g(X)]$$

Proof. Let $\mu = \mathbb{E}[X]$ and let $L_\mu(x) = a + bx$ be the tangent line for the function g at μ, then we have

$L_\mu(\mu) = g(\mu)$. By convexity, we know $g(x) \geq L_\mu(x)$ for all x; thus we have

$$\mathbb{E}[g(X)] \geq \mathbb{E}[L_\mu(X)] = \mathbb{E}[a + bX] = a + b\mu = L_\mu(\mu) = g(\mu)$$

□

Lemma C.6 (MGF of Bounded Variables)**.** The bounded variables is the random variable X with zero mean and with support on some bounded interval $[a, b]$. The MGF of bounded variable is

$$\mathbb{E}_X[e^{tX}] \leq \exp\left(\frac{(b-a)^2 t^2}{2}\right) \tag{C.6}$$

which in turn show that bounded random variables are $(b - a)$ sub-Gaussian.

Proof. Let X be a random variable with zero mean and with support on some bounded interval $[a, b]$, and (note that one can always subtract the means and get a new rv)

$$Y = X - \mathbb{E}[X]$$

using Jensen's inequality and the convexity of $g(x) = e^x$, we have

$$\mathbb{E}_X[e^{tX}] = \mathbb{E}_X\left[e^{t(X - \mathbb{E}[X'])}\right] \leq \mathbb{E}_{X,X'}\left[e^{t(X-X')}\right]$$

now let ε be a Rademacher random variable, and note that the distribution

$$X - X' \overset{d}{=} X' - X \overset{d}{=} \varepsilon(X - X')$$

so we have

$$\mathbb{E}_{X,X'}\left[e^{t(X-X')}\right] = \mathbb{E}_{X,X'}\left[\mathbb{E}_\varepsilon[e^{\varepsilon t(X-X')}]\right] \leq \mathbb{E}_{X,X'}\left[e^{t^2(X-X')^2/2}\right] \leq e^{t^2(b-a)^2/2}$$

with the notice that X is bounded and $(X - X')$ is at most $(b - a)$. In fact, this in turn yields the simple version of Hoeffding's bound. □

Gaussian Random Variables.

Corollary C.7 (Gaussian Tail Bound)**.** Suppose random variable $X \sim N(\mu, \sigma^2)$, the MGF of X is then $\mathbb{E}[e^{tX}] = e^{\mu t + \sigma^2 t^2/2}$. Applying the Chernoff bound, we have one-sided upper bound

$$\mathbb{P}(X - \mu \geq u) \leq \exp\left(-\frac{u^2}{2\sigma^2}\right) \tag{C.7}$$

and *lower tail bound*

$$\mathbb{P}(-X + \mu \geq u) \leq \exp\left(-\frac{u^2}{2\sigma^2}\right)$$

putting these together, we have the *two-sided Gaussian tail bound*:

$$\mathbb{P}(|X - \mu| \geq u) \leq 2\exp\left(-\frac{u^2}{2\sigma^2}\right)$$

Proof. Suppose $X \sim N(\mu, \sigma^2)$, then the MGF of X is

$$\begin{aligned} M_X(t) = \mathbb{E}\left[e^{tX}\right] &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{tx} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{(x-(\mu+\sigma^2 t))^2}{2\sigma^2}} e^{\frac{\sigma^2 t^2}{2}+\mu t} dx \\ &= e^{\mu t + \sigma^2 t^2/2} \end{aligned}$$

or equivalently

$$\mathbb{E}[e^{t(X-\mu)}] = \exp\left(\frac{\sigma^2 t^2}{2}\right) \tag{C.8}$$

to apply the Chernoff bound we then need to compute

$$\inf_{t\geq 0} \frac{e^{\mu t+\sigma^2 t^2/2}}{e^{(u+\mu)t}} = \inf_{t\geq 0} e^{-ut+\sigma^2 t^2/2} = e^{-ut+\sigma^2 t^2/2}|_{t=u/\sigma^2} = e^{-\frac{u^2}{2\sigma^2}}$$

therefore, we obtain one-sided upper tail bound,

$$\mathbb{P}(X - \mu \geq u) \leq \exp\left(-\frac{u^2}{2\sigma^2}\right)$$

□

The Gaussian tail bound is much sharper than Chebyshev's inequality; consider the average of i.i.d. Gaussian random variables, $X_1, \ldots, X_n \sim N(\mu, \sigma^2)$ and we construct the estimate

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i$$

where $\bar{X}_n \sim N(\mu, \sigma^2/n)$, in this case, the Gaussian tail bound is

$$\mathbb{P}\left(\left|\bar{X}_n - \mu\right| \geq t\frac{\sigma}{\sqrt{n}}\right) \leq 2\exp\left(-\frac{t^2}{2}\right)$$

with probability 0.99 ($t = \sqrt{2\ln(1/0.0005)} = 3.25$), that the average $\bar{X}_n$ is within $3.25\sigma/\sqrt{n}$. More generally, with probability at least $1 - \delta$

- Chebyshev tells us that
$$|\bar{X}_n - \mu| \leq \frac{\sigma}{\sqrt{n\sigma}}$$
- Chernoff tail bound tells us that
$$|\bar{X}_n - \mu| \leq \sigma\sqrt{\frac{2\ln(2/\delta)}{n}}$$

Sub-Gaussian Random Variables.

Corollary C.8 (Sub-Gaussian Tail Bound)**.** Formally, a random variable X with mean μ is called σ-sub-Gaussian if there exists a positive number σ such that

$$\mathbb{E}[e^{t(X-\mu)}] \leq \exp\left(\frac{\sigma^2 t^2}{2}\right) \tag{C.9}$$

Roughly, these are random variables whose tails decay faster than a Gaussian. Similar to Gaussian tail bound, here we can derive the two-sided sub-Gaussian tail bound

$$\mathbb{P}(|X-\mu| \geq u) \leq 2\exp\left(-\frac{u^2}{2\sigma^2}\right) \tag{C.10}$$

Now, suppose we have n i.i.d. σ sub-Gaussian random variables $X_1, X_2, \ldots, X_n$, again

$$\bar{X}_n = \frac{1}{n}\sum_i X_i$$

by independence we have

$$\mathbb{E}\left[e^{t(\bar{X}_n-\mu)}\right] = \mathbb{E}\left[e^{\frac{t}{n}\sum_i (X_i-\mu)}\right] = \prod_{i=1}^{n} \mathbb{E}[e^{\frac{t}{n}(X_i-\mu)}] \leq \prod_{i=1}^{n} e^{\frac{\sigma^2 t^2}{2n^2}} = \exp\left(\frac{\sigma^2 t^2}{2n}\right)$$

alternatively, $\bar{X}_n$ is $\sigma/\sqrt{n}$ sub-Gaussian, this yields the tail bound for the average of sub-Gaussian rvs:

$$\mathbb{P}\left(\left|\bar{X}_n-\mu\right| \geq k\frac{\sigma}{\sqrt{n}}\right) \leq 2\exp\left(-\frac{k^2}{2}\right)$$

Exponential Random Variables

Theorem C.9 (Exponential Tail Bound)**.** Suppose that we have $X_1, \ldots, X_n$ which are each $\sigma_1, \ldots, \sigma_n$ sub-Gaussian; they are not identically distributed, but using just *independence*, one can verify that the average $\bar{X}_n$ is σ sub-Gaussian where

$$\sigma = \frac{1}{n}\sqrt{\sum_{i=1}^{n}\sigma_i^2}$$

this yields the *exponential tail inequality*

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}(X_i-\mu_i)\right| \geq t\right) \leq \exp\left(-\frac{t^2}{2\sigma^2}\right) \tag{C.11}$$

note the these random variables still need to be independent.

C.4 Hoeffding's Inequality

Here we use the information of bounded variable (first-order info) to bound the MGF of random variable, then we utilize the methodds of Chernoff bound.

Theorem C.10 (Hoeffding's Inequality)**.** Suppose $X_1, \ldots, X_n$ are i.i.d bounded random variables, with $X_i \in [a, b]$, then the sample average, $\bar{X}_n = \frac{1}{n}\sum_i X_i$ has the bound

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{k=1}^{n} X_k - \mu\right| \geq t\right) \leq 2\exp\left(-\frac{2nt^2}{(b-a)^2}\right) \tag{C.12}$$

The Hoeffding's inequality tells us that, with probability at least $1-\delta$,

$$\left|\frac{1}{n}\sum_{k=1}^{n} X_k - \mu\right| \le (b-a)\sqrt{\frac{\ln(2/\delta)}{2n}} \tag{C.13}$$

where $\hat{\mu} = \bar{X}_n$ is the sample-average estimator of mean μ.

Proof. Suppose the random variable X has mean μ and is bounded by $[a,b]$. The logarithmic moment generating function of X is then

$$\varphi(s) = \log \mathbb{E}\left[e^{s(X-\mu)}\right]$$

The usual derivatives of $\varphi(s)$ is then

$$\begin{aligned}
\varphi'(s) &= \frac{\mathbb{E}[(X-\mu)e^{s(X-\mu)}]}{\mathbb{E}[e^{s(X-\mu)}]} \\
\varphi''(s) &= \frac{\mathbb{E}[(X-\mu)^2 e^{s(X-\mu)}]}{\mathbb{E}[e^{s(X-\mu)}]} - \left(\frac{\mathbb{E}[(X-\mu)e^{s(X-\mu)}]}{\mathbb{E}[e^{s(X-\mu)}]}\right)^2 \\
&= \frac{\int_a^b (x-\mu)^2 e^{s(x-\mu)} dP(x)}{\int_a^b e^{s(x-\mu)} dP(x)} - \left(\frac{\int_a^b (x-\mu) e^{s(x-\mu)} dP(x)}{\int_a^b e^{s(x-\mu)} dP(x)}\right)^2
\end{aligned}$$

where we assume $P(x)$ is the distribution of X. It is essential to notice that $\varphi''(s)$ is the varaince of some random variable $\tilde{X} \in [a,b]$ with the distribution proportional to $e^{s(x-\mu)}dP(x)$. Therefore, we can bound the variance of $\tilde{X}$ as

$$\mathrm{Var}(\tilde{X}) = \inf_{\mu \in [a,b]} \mathbb{E}[\tilde{X}-\mu]^2 \le \mathbb{E}\left[\tilde{X} - \frac{a+b}{2}\right]^2 \le \frac{(b-a)^2}{4}$$

for any s almost surely. Since $\varphi(0) = 0$ and $\varphi'(0) = 0$, the Taylor's expansion with Lagrange remainder of $\varphi(s)$ at point $s = 0$ satisfies

$$\varphi(s) = \varphi(0) + \frac{\varphi'(0)}{1!}s + \frac{\varphi''(\xi)}{2!}s^2 \le \frac{(b-a)^2}{8}s^2 \quad \text{almost surely}$$

where $\xi \in [0,s]$. That means

$$\mathbb{E}\left[e^{s(X-\mu)}\right] \le \exp\left(\frac{(b-a)^2}{8}s^2\right) \tag{C.14}$$

Now we have complete the key part of the proof. Next, recall the Markov's inequality for any non-negative random X and $\varepsilon > 0$,

$$\begin{aligned}
\mathbb{P}(\bar{X}_n - \mu \ge t) &= \mathbb{P}(e^{s(\bar{X}_n-\mu)} \ge e^{st}) \\
&\le \inf_s \; e^{-st}\mathbb{E}\left[e^{s(\bar{X}_n-\mu)}\right] \\
&= \inf_s \; e^{-st}\prod_{i=1}^{n}\mathbb{E}\left[e^{\frac{s}{n}(X_i-\mu)}\right] \\
&\le \inf_s \; e^{-st}\prod_{i=1}^{n}\exp\left(\frac{s^2(b-a)^2}{8n}\right) \\
&= \inf_s \; \exp\left(-st + \frac{s^2(b-a)^2}{8n}\right) \\
&= \exp\left(-\frac{2nt^2}{(b-a)^2}\right), \qquad s = \frac{4nt}{(b-a)^2}
\end{aligned}$$

Repeating this in the other direction we get

$$\mathbb{P}\big(|\bar{X}_n - \mu| \geq t\big) \leq 2\exp\left(-\frac{2nt^2}{(b-a)^2}\right)$$

□

C.5 Bernstein's Inequality

The Hoeffding's bound depended only on the bounds of the random variable but not explicityly on the variance. The bound $b-a$, provides a (possibly loss) upper bound on the standard deviation. One might at least hope that if the random variables were bounded, and additionally had small variance, we might be able to imporve Hoeffding's bound.

Theorem C.11 (Berstein's Inequality)**.** Suppose we have $X_1, \ldots, X_n$ which were i.i.d from a distribution with mean μ, bounded suppport $[a,b]$, with variance $\mathbb{E}(X-\mu)^2 = \sigma^2$, then

$$\mathbb{P}\left(\left|\frac{1}{n}\sum_{k=1}^{n} X_k - \mu\right| \geq t\right) \leq 2\exp\left(-\frac{nt^2}{2\sigma^2 + 2(b-a)t/3}\right) \tag{C.15}$$

The inequality implies that, with probability at least $1-\delta$,

$$\left|\frac{1}{n}\sum_{k=1}^{n} X_k - \mu\right| \leq \sigma\sqrt{\frac{2\ln(1/\delta)}{n}} + \frac{2(b-a)\ln(1/\delta)}{3n}$$

Proof. Using the Taylor's expansion of the exponential, we can bound the moment generating function of X by

$$\begin{aligned}
\mathbb{E}\left[e^{s(X-\mu)}\right] &= 1 + s\mathbb{E}(X-\mu) + \sum_{k=2}^{\infty}\frac{s^k}{k!}\mathbb{E}(X-\mu)^k = 1 + \sum_{k=2}^{\infty}\frac{s^k}{k!}\mathbb{E}(X-\mu)^k \\
&\leq 1 + \sum_{k=2}^{\infty}\frac{s^k}{k!}\mathbb{E}\left[|X-\mu|^{k-2}|X-\mu|^2\right] \\
&\leq 1 + \sum_{k=2}^{\infty}\frac{s^k}{k!}\mathbb{E}|X-\mu|^{k-2}\sigma^2 \qquad \text{(Cauchy-Schwartz inequality)} \\
&= 1 + \frac{\sigma^2}{c^2}\sum_{k=2}^{\infty}\frac{s^k}{k!}, c^k \qquad \text{let } c = \mathbb{E}|X-\mu| \leq (b-a) \\
&= 1 + \frac{\sigma^2}{c^2}(e^{sc} - 1 - sc) \\
&\leq \exp\left(\frac{\sigma^2}{c^2}(e^{sc} - 1 - sc)\right)
\end{aligned}$$

With $\sigma^2 = \mathrm{Var}(X_i)$, we have

$$\begin{aligned}
\mathbb{P}\left(\bar{X}_n - \mu \geq t\right) &= \mathbb{P}\left(e^{s(\bar{X}_n - \mu)} \geq e^{st}\right) \qquad \text{(Markov's inequality)} \\
&\leq \inf_s \; e^{-st}\mathbb{E}\left[e^{s(\bar{X}_n-\mu)}\right] \\
&= \inf_s e^{-st} \prod_{i=1}^n \mathbb{E}\left[e^{\frac{s}{n}(X_i-\mu)}\right] \\
&\leq \inf_s \; e^{-st} \prod_{i=1}^n \exp\left(\frac{\sigma^2}{c^2}\left(e^{\frac{sc}{n}} - 1 - \frac{sc}{n}\right)\right) \\
&= \inf_s \; \exp\left(-st + \frac{\sigma^2}{c^2}\left(ne^{\frac{sc}{n}} - n - sc\right)\right) \\
&= \exp\left(\frac{nt}{c} - \frac{nt}{c}\ln\left(1 + \frac{tc}{\sigma^2}\right) - \frac{n\sigma^2}{c^2}\ln\left(1 + \frac{tc}{\sigma^2}\right)\right), \qquad s = \frac{n}{c}\ln\left(1 + \frac{tc}{\sigma^2}\right) \\
&= \exp\left(-\frac{n\sigma^2}{c^2}\Big((1+\alpha)\ln(1+\alpha) - \alpha\Big)\right), \qquad \alpha = \frac{tc}{\sigma^2} = \frac{t(b-a)}{\sigma^2}
\end{aligned}$$

With the knowing that

$$(1+\alpha)\ln(1+\alpha) - \alpha \geq \frac{\alpha^2}{2 + 2\alpha/3}$$

we have

$$\mathbb{P}\left(|\bar{X}_n - \mu| \geq t\right) \leq \exp\left(-\frac{nt^2}{2\sigma^2 + 2(b-a)t/3}\right)$$

□

C.6 McDiarmid's Inequality

So far we have focused on the concentration of averages. A natural question is whether other functions of i.i.d. random variables also show exponential concentration. It turns out that many other functions do concentrate sharply, and roughly the main property of the function that we need is that if we change the value of one random variable the function does not change dramatically.

Theorem C.12 (McDiarmid's Inequality)**.** Suppose we have i.i.d random variables $X_1, \dots, X_n$ where each $X_i \in \mathbb{R}^n$. We have a Lipschitz function $f : \mathbb{R}^n \to \mathbb{R}$, that satisfies the property that:

$$|f(x_1, \dots, x_{k-1}, x_k, x_{k+1}, \dots, x_n) - f(x_1, \dots, x_{k-1}, x'_k, x_{k+1}, \dots, x_n)| \leq L_k$$

for every $x, x' \in \mathbb{R}^n$. Then for any $t \geq 0$

$$\mathbb{P}\big(|f(X_1, \dots, X_n) - \mathbb{E}f(X_1, \dots, X_n)| \geq t\big) \leq 2\exp\left(-\frac{2t^2}{\sum_{k=1}^n L_k^2}\right) \tag{C.16}$$

Proof. The proof generalizes Hoeffding's inequality, which corresponds to $f(x) = \frac{1}{n}\sum_{i=1}^n x_i$. Now, we introduce the random variables V_k for $k = 1, \dots, n$,

$$V_k = \mathbb{E}[f(X_1, \dots, X_n) \mid X_1, \dots, X_k] - \mathbb{E}[f(X_1, \dots, X_n) \mid X_1, \dots, X_{k-1}]$$

By the law of iterated expectation, we have

$$\mathbb{E}[V_k \mid X_1, \dots, X_{k-1}] = \mathbb{E}[f(X_1, \dots, X_n) \mid X_1, \dots, X_{k-1}] - \mathbb{E}[f(X_1, \dots, X_n) \mid X_1, \dots, X_{k-1}] = 0$$

and in the mean time,

$$\sum_{k=1}^{n} V_k = f(X_1, \dots, X_n) - \mathbb{E}f(X_1, \dots, X_n)$$

Since $|V_k| \leq L_k$ almost surley, V_k is also an bounded variable. Using the exact method as in the proof of Hoeffding's inequality, we have

$$\mathbb{E}\left[e^{sV_k}\right] \leq \exp\left(\frac{L_k^2}{8}s^2\right)$$

Then

$$\begin{aligned}
\mathbb{P}\left(\sum_{k=1}^{n} V_k \geq t\right) &= \mathbb{P}\left(e^{s\sum_{k=1}^{n} V_k} \geq e^{st}\right) \\
&\leq \inf_s \; e^{-st}\mathbb{E}\left[e^{s\sum_{k=1}^{n} V_k}\right] \qquad \text{(Markov's inequality)} \\
&= \inf_s \; e^{-st}\prod_{k=1}^{n}\mathbb{E}\left[sV_k\right] \\
&\leq \inf_s \; e^{-st}\prod_{k=1}^{n}\exp\left(\frac{L_k^2}{8}s^2\right) \\
&= \inf_s \exp\left(-st + \frac{\sum_{k=1}^{n} L_k^2}{8}s^2\right) \\
&= \exp\left(-\frac{2t^2}{\sum_{k=1}^{n} L_k^2}\right), \qquad s = \frac{4t}{\sum_{k=1}^{n} L_k^2}
\end{aligned}$$

□

C.7 Expectation of the Maximum

Theorem C.13 (Expectation of the Maximum)**.** If $Z_1, \dots, Z_n$ are (potentially dependent) random variables which are σ-sub-Gaussian, then

$$\mathbb{E}[\max\{Z_1 - \mathbb{E}[Z_1], \dots, Z_n - \mathbb{E}[Z_n]\}] \leq \sqrt{2\sigma^2 \log n}$$

Proof. By using the Jensen's inequality for logarithm, which is concave, we have

$$\begin{aligned}
\mathbb{E}\Big[\max\left\{Z_1 - \mathbb{E}[Z_1], \dots, Z_n - \mathbb{E}[Z_n]\right\}\Big] &\leq \frac{1}{t}\log\mathbb{E}\left[e^{t\max\{Z_1-\mathbb{E}[Z_1],\dots,Z_n-\mathbb{E}[Z_n]\}}\right] \qquad \text{(by Jensen's inequality)} \\
&= \frac{1}{t}\log\mathbb{E}\left[\max\left\{e^{t(Z_1-\mathbb{E}[Z_1])}, \dots, e^{t(Z_n-\mathbb{E}[Z_n])}\right\}\right] \\
&\leq \frac{1}{t}\log\mathbb{E}\left[e^{t(Z_1-\mathbb{E}[Z_1])} + \cdots + e^{t(Z_n-\mathbb{E}[Z_n])}\right] \qquad \text{(bounding the max by the sum)} \\
&\leq \frac{1}{t}\log\left(ne^{\sigma^2t^2/2}\right) = \frac{\log n}{t} + \sigma^2\frac{t}{2} \qquad \text{(by sub-Gaussian property)}
\end{aligned}$$

Since such inequality is hold for any $t \in \mathbb{R}$, then we can minimize over t and get $t = \sigma^{-1}\sqrt{2\log n}$. Thus

$$\mathbb{E}\Big[\max\big\{Z_1 - \mathbb{E}[Z_1], \dots, Z_n - \mathbb{E}[Z_n]\big\}\Big] \le \sigma\sqrt{2\log n}$$

□

D Concentration for Matrices

D.1 Matrix Analysis

D.1.1 Matrix Functions

Consider a function $f : \mathbb{R} \to \mathbb{R}$. We define a map on diagonal matrices by applying the function to each diagonal entry. We then extend f to a function on Hermitian matrices using the eigenvalue decomposition:

$$f(A) := Qf(\Lambda)Q^* \tag{D.1}$$

where $A = Q\Lambda Q^*$. The *spectral mapping theorem* states that each eigenvalue of $f(A)$ is equal to $f(\lambda)$ for some eigenvalue λ of A. This point is obvious from our definition.

Standard inequalities for real functions typically do not have parallel versions that hold for the semi-definite ordering. Nevertheless, there is one type of relation for real functions that always extends to the semi-definite setting.

$$f(a) \le g(a) \quad \forall\ a \in I \quad \Longrightarrow \quad f(A) \preceq g(A) \tag{D.2}$$

when the eigenvalues of A lie in I. We sometimes refer to this as the *transfer rule*.

D.1.2 Matrix Exponential

The exponential of an Hermitian matrix A can be defined by applying (D.1) with the function $f(x) = e^x$. Alternatively, we may use the power series expansion

$$\exp(A) := I + \sum_{p=1}^{\infty} \frac{A^p}{p!}$$

The exponential of an Hermitian matrix H is always **positive definite** from the spectral mapping theorem. Here is a sketch proof,

$$x^\top e^H x = x^\top e^{H/2} e^{H/2} x = \left(e^{H/2}x\right)^\top \left(e^{H/2}x\right) = \left|\left|e^{H/2}x\right|\right|_2^2 \ge 0 \tag{D.3}$$

because of the eigenvalue decomposition of Hermitian matrix. On account of the transfer rule (D.2), the matrix exponential satisfies some simple semidefinite relations that we collect here. For each Hermitian matrix A, it holds that

$$\begin{gathered} I + A \preceq e^A \\ \cosh(A) \preceq e^{A^2/2} \end{gathered} \tag{D.4}$$

We often work with the trace of the matrix exponential, $\operatorname{tr}\exp : A \mapsto \operatorname{tr} e^A$. The trace exponential function is **convex**. It is also monotone with respect to the semi-definite order:

$$A \preceq H \quad \Rightarrow \quad \operatorname{tr} e^A \le \operatorname{tr} e^H \tag{D.5}$$

The matrix exponential does not convert sums into products, but the trace exponential has a related property that serves as a limited substitue. The Golden-Thompson inequality states that

$$\operatorname{tr} e^{A+H} \leq \operatorname{tr}\left(e^A e^H\right) \quad \text{for all Hermitian } A, H \tag{D.6}$$

The obvious generalization of the bound (D.6) to three matrices is **false**. The pperator monotone functions and operator convex functions are depressingly rare. In particular, the matrix exponential does not belong to either.

D.1.3 Matrix Logarithm

We define the matrix logarithm as the functional inverse of the matrix exponential

$$\log e^A := A \quad \text{for all Hermitian } A$$

This formular determines the logarithm on the positive definite cone, which is adequate for our purposes.

The matrix logarithm interacts beautifully with the semidefinite order. Indeed, the logarithm is opeartor monotone:

$$0 \prec A \preceq H \quad \Longrightarrow \quad \log(A) \preceq \log(H) \tag{D.7}$$

The logarithm is also operator concave:

$$\alpha \log A + (1-\alpha)\log H \preceq \log(\alpha A + (1-\alpha)H) \tag{D.8}$$

for all PD A, H and $\alpha \in [0,1]$.

D.1.4 Expectation and the Semidefinite Order

Since the expectation of a random matrix can be viewed as a convex combination and the PSD cone is convex, expectation preserves the semi-definite order:

$$X \preceq Y \text{ almost surely} \quad \Longrightarrow \quad \mathbb{E}[X] \preceq \mathbb{E}[Y] \tag{D.9}$$

Every operator convex function admits an operator Jensen's inequality. In particular, the matrix square is operator convex, which implies that

$$(\mathbb{E}X)^2 \preceq \mathbb{E}X^2 \tag{D.10}$$

D.1.5 Matrix Martingales

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a master probability space. Consider a filtration $\{\mathcal{F}_k\}$ contained in the master sigma algebra:

$$\mathcal{F}_0 \subset \mathcal{F}_1 \subset \cdots \subset \mathcal{F}_\infty \subset \mathcal{F}$$

Given such a filtration, we define the conditional expectation $\mathbb{E}_k[\cdot] := \mathbb{E}[\cdot \mid \mathcal{F}_k]$. A sequence of $\{X_k\}$ of random matrices is adapated to the filtration when each X_k is measurable with respect to $\mathcal{F}_k$. Loosely speaking, an adapted sequence is one where the present depends only upon the past.

An adapted sequence $\{Y_k\}$ of Hermitian matrices is called a matrix martingale when

$$\mathbb{E}_{k-1}[Y_k] = Y_{k-1} \quad \text{and} \quad \mathbb{E}||Y_k|| < \infty \quad \text{for} \quad k = 1, 2, 3, \ldots$$

We obtain a scalar martingale if we track any fixed coordinate of a matrix martingale $\{Y_k\}$. Given a matrix martingale $\{Y_k\}$, we can construct the difference sequence

$$X_k := Y_k - Y_{k-1} \quad \text{for} \quad k = 1, 2, 3$$

Note that the difference sequence is conditionally zero mean, $\mathbb{E}_{k-1} X_k = 0$.

D.2 Tail Bounds via the Matrix Laplace Transform Method

D.2.1 Matrix Moments and Cumulants

Consider a random Hermitian matrix X that has momens of all orders. By analogy with the classical scalar definitions, we may construct matrix extensions of the moment-generating function (MGF) and the cumulant-generating function (CGF):

$$M_X(\theta) := \mathbb{E} e^{\theta X} \quad \text{and} \quad C_X(\theta) := \log\left(\mathbb{E} e^{\theta X}\right) \tag{D.11}$$

We admit the possibility that these expectations do not exist for all value of θ. The matrix MGF and CGF have formal power series expansions:

$$M_X(\theta) = I + \sum_{p=1}^{\infty} \frac{\theta^p}{p!} \cdot \mathbb{E}[X^p] \quad \text{and} \quad C_X(\theta) = \sum_{p=1}^{\infty} \frac{\theta^p}{p!} \cdot \Psi_p$$

The coefficients $\mathbb{E}[X^p]$ are caled matrix moments, and we refer to Ψ_p as a matrix cumulant. The first cumulant is the mean and the second cumulant is the variance

$$\Psi_1 = \mathbb{E}[X] \quad \text{and} \quad \Psi_2 = \mathbb{E}[X^2] - (\mathbb{E}X)^2$$

Higher-order cumulants are harder to write down and interpret.

D.2.2 Laplace Transform Method

Proposition D.1 (The Laplace Transform Method)**.** Let Y be a random Hermitian matrix. Then for all $t \in \mathbb{R}$,

$$\mathbb{P}\left(\lambda_{\max}(Y) \geq t\right) \leq \inf_{\theta > 0} \left\{ e^{-\theta t} \cdot \mathbb{E}\left[\operatorname{tr} e^{\theta Y}\right] \right\} \tag{D.12}$$

In words, we can control tail probabilities for the maximum eigenvalue of a random matrix by producing a bound for the trace of the matrix MGF.

Proof. Fix a positive number θ, we have the chain of relations

$$\mathbb{P}(\lambda_{\max} \geq t) = \mathbb{P}(\lambda_{\max}(\theta Y) \geq \theta t) = \mathbb{P}\left(e^{\lambda_{\max}(\theta Y)} \geq e^{\theta t}\right) \leq e^{-\theta t} \cdot \mathbb{E} e^{\lambda_{\max}(\theta Y)}$$

The first identity uses the homogeneity of the maximum eigenvalue map, and the second relies on the monotonicity of the scalar exponential function; the third relation is Markov's inequality. To bound the exponential, note that

$$e^{\lambda_{\max}(\theta Y)} = \lambda_{\max}\left(e^{\theta Y}\right) \leq \operatorname{tr} e^{\theta Y}$$

The identity is the spectral mapping theorem; the inequality holds because the exponential of an Hermitian matrix is positive definite and the maximum eigenvalue of a positive definitie matrix is dominated by the trace. Combine the latter two relations to reach

$$\mathbb{P}(\lambda_{\max}(Y) \geq t) \leq e^{-\theta t} \cdot \mathbb{E}\left[\operatorname{tr} e^{\theta Y}\right]$$

This inequality holds for any positive θ, wo we take an infimum to complete the proof. □

D.2.3 Failure of the Matrix MGF

In the scalar setting, the Laplace transform method is very effective for studying sums of independent random variables because the MGF decomposes. Consider an independent sequence $\{Z_k\}$ of real random variables. We see that the scalar MGF of the sum satisfies a multiplication rule

$$M_{\sum X_k}(\theta) = \mathbb{E} \exp\left(\sum_k \theta X_k\right) = \mathbb{E} \prod_k e^{\theta X_k} = \prod_k \mathbb{E} e^{\theta X_k} = \prod_k M_{X_k}(\theta) \tag{D.13}$$

This calculation relies on the fact that the scalar exponential function converts sums to products, a property th matrix exponential does not share. As a consequence, there is no immediate analog of (D.13) in the matrix setting

D.2.4 A Concave Trace Function

Theorem D.1 (Lieb)**.** Fix a Hermitian matrix H. The function

$$f : A \mapsto \operatorname{tr} \exp(H + \log A)$$

is **concave** on the positive definite cone.

We require a simple but powerful corollary of Lieb's theorem. This result describes how expectation interacts with the trace exponential.

Corollary D.2. Let H be a fixed Hermitian matrix, and let X be a random Hermitian matrix. Then

$$\mathbb{E}\left[\operatorname{tr} \exp(H + X)\right] \leq \operatorname{tr} \exp\left(H + \log\left(\mathbb{E} e^X\right)\right)$$

Proof. Define the random matrix $Y = e^X$, and calculate that

$$\mathbb{E}[\operatorname{tr} \exp(H + X)] = \mathbb{E}[\operatorname{tr} \exp(H + \log Y)] \leq \operatorname{tr} \exp(H + \log(\mathbb{E} Y)) = \operatorname{tr} \exp\left(H + \log\left(\mathbb{E} e^X\right)\right)$$

The first identity follows from the definition of the matrix logarithm because Y is always PD. Lieb's result, ensures that the trace function is concave in Y, so we may invoke Jensen's inequality to draw the expectation inside the logarithm. □

D.2.5 Subadditivity of the Matrix CGF

Although the multiplication rule (D.13) of MGF is a dead end in the matrix case, the scalar CGF has a related property that submits to generalization. For an independent family $\{X_k\}$ or real random variables, the scalar CGF is additive:

$$C_{\sum_K X_k}(\theta) = \log \mathbb{E} \exp\left(\sum_k \theta X_K\right) = \sum_k \log \mathbb{E} e^{\theta X_k} = \sum_k C_{X_k}(\theta) \tag{D.14}$$

where the second identity comes from (D.13) when take logarithms.

One key insight is that Corollary D.2 offers a completely satisfactory way to extend the addition rule (D.14) for scalar CGF's the matrix setting. We have the following result.

Lemma D.3 (Subadditiveity of Matrix CGF's)**.** Consider a finite sequence $\{X_k\}$ of independent, random, Hermitian matrices. Then

$$\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right] \le \operatorname{tr}\exp\left(\sum_k \log \mathbb{E}\left[e^{\theta X_k}\right]\right) \quad \forall\ \theta \in \mathbb{R} \tag{D.15}$$

Proof. It does not harm to assume $\theta = 1$. Let $\mathbb{E}_k$ denote the expectation, conditioned on $X_1, \dots, X_k$. Abbreviate

$$C_k := \log \mathbb{E}_{k-1}\left[e^{X_k}\right] = \log \mathbb{E}\left[e^{X_k}\right] = X_k$$

where the equality holds because the family $\{X_k\}$ is independent. We see that

$$\begin{aligned}
\mathbb{E} \operatorname{tr}\exp\left(\sum_{k=1}^{n} X_k\right) &= \mathbb{E}_0 \cdots \mathbb{E}_{n-1} \operatorname{tr}\exp\left(\sum_{k=1}^{n-1} X_k + X_n\right) \\
&\le \mathbb{E}_0 \cdots \mathbb{E}_{n-2} \operatorname{tr}\exp\left(\sum_{k=1}^{n} X_k + \log \mathbb{E}_{n-1}\left[e^{X_n}\right]\right) \quad \text{by Corollary D.2} \\
&= \mathbb{E}_0 \cdots \mathbb{E}_{n-2} \operatorname{tr}\exp\left(\sum_{k=1}^{n-2} + X_{n-1} + C_n\right) \\
&\le \mathbb{E}_0 \cdots \mathbb{E}_{n-3} \operatorname{tr}\exp\left(\sum_{k=1}^{n-2} X_k + C_{n-1} + C_n\right) \\
&\dots \\
&\le \operatorname{tr}\exp\left(\sum_{k=1}^{n} C_k\right)
\end{aligned}$$

□

To make the parallel with the addition rule (D.14) clearer, we can rewrite the conclusion of this lemma in the form

$$\operatorname{tr}\exp\left(C_{\sum_k X_K}(\theta)\right) \le \operatorname{tr}\exp\left(\sum_k C_{X_k}(\theta)\right) \tag{D.16}$$

by applyting the definition of the matrix CGF.

D.2.6 Tail Bounds of Independent Sums

This section contains abstract tail bounds for the sum of independent random matrices. Later, we will specialize these results to some specific situations. We begin with a very general inequality, which is the progenitor of other results.

Theorem D.4 (Master Tail Bound for Independence Sums)**.** Consider a finite sequence $\{X_k\}$ of independent, random, Hermitian matrices. For all $t \in \mathbb{R}$

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq \inf_{\theta \geq 0}\left\{e^{-\theta t} \cdot \operatorname{tr}\exp\left(\sum_k \log \mathbb{E}\left[e^{\theta X_k}\right]\right)\right\} \tag{D.17}$$

Proof. From Laplace transform bound, for random Hermitian matrice Y, we have

$$\mathbb{P}(\lambda_{\max}(Y) \geq t) \leq \inf_{\theta > 0}\left\{e^{-\theta t} \cdot \mathbb{E}\left[\operatorname{tr}\exp(\theta Y)\right]\right\}$$

Notice that the sum of i.i.d random Hermitian matrices $\sum_k X_k$ is still a random Hermitian matrice, and hence we have

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq \inf_{\theta > 0}\left\{e^{-\theta t} \cdot \mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right]\right\}$$

By applying the subadditivity of matrix CGF in Lemma D.3, we have

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq \inf_{\theta > 0}\left\{e^{-\theta t} \cdot \operatorname{tr}\exp\left(\sum_k \log \mathbb{E}\left[e^{\theta X_k}\right]\right)\right\}$$

□

Corollary D.5. Consider a finite sequence $\{X_k\}$ of independent, random, self-adjoint matrices with dimension d. Assume there is a function $g : (0, \infty) \to [0, \infty]$ and a sequence $\{A_k\}$ of fixed Hermitian matrices that satisfy the relations

$$\mathbb{E}\left[e^{\theta X_k}\right] \preceq e^{g(\theta) \cdot A_k} \tag{D.18}$$

for $\theta > 0$. Define the scale parameter $\rho := \lambda_{\max}(\sum_k A_k)$. Then for all $t \in \mathbb{R}$,

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq d \cdot \inf_{\theta > 0}\left\{e^{-\theta t + g(\theta) \cdot \rho}\right\} \tag{D.19}$$

Proof. The hypothesis implies that

$$\log \mathbb{E}\left[e^{\theta X_k}\right] \preceq g(\theta) \cdot A_k$$

for $\theta > 0$ becasue of the property that the matrix logarithm is operator monotone. Recall that the trace exponential is monotone with respect to the semidefinite order, i.e.

$$A \preceq H \quad \Rightarrow \quad \operatorname{tr} e^A \preceq \operatorname{tr} e^H$$

As a consequence, we can introduce such relation into the master inequality (D.17), that is, for each $\theta > 0$

$$\begin{aligned}\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) &\leq e^{-\theta t} \cdot \operatorname{tr}\exp\left(\sum_k \log \mathbb{E}\left[e^{\theta X_k}\right]\right) \\ &\leq e^{-\theta t} \cdot \operatorname{tr}\exp\left(g(\theta)\sum_k A_k\right) \\ &\leq e^{-\theta t} \cdot d \cdot \lambda_{\max}\left(\exp\left(g(\theta)\sum_k A_k\right)\right) \\ &= d \cdot e^{-\theta t} \cdot \exp\left(g(\theta) \cdot \lambda_{\max}\left(\sum_k A_k\right)\right)\end{aligned}$$

The third inequality holds because the trace of a PD matrix, such as the exponential of matrix), is bounded by the dimension d times the maximum eigenvalue. The last line depends on the spectral mapping theorem and the fact that the function g is nonnegative. Identify the quantity $\rho := \lambda_{\max}(\sum_k A_k)$, and take the infimum over positive θ to reach the conclusion. □

Remark D.1 (Minimum Eigenvalue)**.** We can study the minimum eigenvalue of a sum of random Hermitian matrices because $\lambda_{\min}(X) = -\lambda_{\max}(-X)$. As a result

$$\mathbb{P}\left(\lambda_{\min}\left(\sum_k X_k\right) \leq t\right) = \mathbb{P}\left(\lambda_{\max}\left(\sum_k -X_k\right) \geq -t\right)$$

Remark D.2 (Maximum Singular Value)**.** We can also analyze the maximum singular value of a sum of random rectangular matrices B by applying these results to the Hermitian dilation, that is

$$\varphi(B) := \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix}$$

For a finite sequence $\{Z_k\}$ of independent, random, rectangular matrices, we have

$$\mathbb{P}\left(\left\|\sum_k Z_k\right\| \geq t\right) = \mathbb{P}\left(\lambda_{\max}\left(\sum_k \varphi(Z_k)\right) \geq t\right)$$

and the property that dilation is real-linear. This device allows us to extend most of the tail bounds in this paper to rectangular matrices.

D.3 Matrix Gaussian and Rademacher

We begin with the scalar case. Consider a finite sequence $\{a_k\}$ of real numbers and a finite sequence $\{\gamma_k\}$ of independent standard Gaussian variables. We have the probability inequality

$$\mathbb{P}\left(\sum_k a_k \gamma_k \geq t\right) \leq \exp\left(-\frac{t^2}{2\sigma^2}\right) \tag{D.20}$$

where $\sigma^2 := \sum_k a_k^2$. This result testifies that a Gaussian series with real coefficients satisfies a normal-type tail bound where the variance is controlled by the sum of the squared coefficients. The relation follows easily from the scalar Laplace transform method.

Lemma D.6 (Rademacher and Gaussian MGF's)**.** Suppose that A is an Hermitian matrix. Let σ be a Rademacher random variable, and let γ be a standard normal random variable. Then

$$\mathbb{E}\left[e^{\sigma\theta A}\right] \preceq e^{\theta^2 A^2/2} \quad \text{and} \quad \mathbb{E}\left[e^{\gamma\theta A}\right] = \mathbb{E}e^{\theta^2 A^2/2} \quad \theta \in \mathbb{R} \tag{D.21}$$

Proof of Lemma D.6. Absorbing θ into A, we may assume $\theta = 1$ in each case. We begin with the Rademacher MGF. By direct calculation,

$$\mathbb{E}e^{\varepsilon A} = \cosh(A) \preceq e^{A^2/2}$$

where the second realtion is (D.4). For the Gaussian case, recall that the moments of a standard normal variable satisfy

$$\mathbb{E}[\gamma^{2p+1}] = 0 \quad \text{and} \quad \mathbb{E}[\gamma^{2p}] = \frac{(2p)!}{p!2^p} \quad p = 0, 1, 2\ldots$$

Therefore,

$$\mathbb{E}e^{\gamma A} = I + \sum_{p=1}^{\infty} \frac{\mathbb{E}[\gamma^{2p}]A^{2p}}{(2p)!} = I + \sum_{p=1}^{\infty} \frac{(A^2/2)^p}{p!} = e^{A^2/2}$$

□

Theorem D.7 (Matrix Gaussian and Rademacher Series)**.** Consider a finite sequence $\{A_k\}$ of fixed (non-random) Hermitian matrices with dimension dm, and let $\{\gamma_k\}$ be a finite sequence of independent standard normal variables. Compute the variance parameter $\sigma^2 := ||\sum_k A_k^2||_2$. Then, for all $t \geq 0$

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k \gamma_k A_k\right) \geq t\right) \leq d \cdot \exp\left(-\frac{t^2}{2\sigma^2}\right) \tag{D.22}$$

In particular,

$$\mathbb{P}\left(\left\|\sum_k \gamma_k A_k\right\|_2 \geq t\right) \leq 2d \cdot \exp\left(-\frac{t^2}{2\sigma^2}\right) \tag{D.23}$$

The same bounds hold when we replace $\{\gamma_k\}$ by a finite sequence of independent Rademacher random variables.

Proof of Theorem D.7. Let ξ_k be a finite sequence of independent standard normal variables or independent Rademacher variables. Invoke Lemma (D.6) to obtain

$$\mathbb{E}e^{\xi_k \theta A_k} \preceq e^{g(\theta)A_k^2}$$

where $g(\theta) := \theta^2/2$ for $\theta > 0$. Recall that

$$\sigma^2 = \left\|\sum_k A_k^2\right\| = \lambda_{\max}\left(\sum_k A_k^2\right)$$

Corollary D.5 delivers

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k \xi_k A_k\right) \geq t\right) \leq d \cdot \inf_{\theta > 0} e^{-\theta t + g(\theta)\cdot\sigma^2} = d \cdot e^{-t^2/2\sigma^2} \tag{D.24}$$

where the infimum is attained when $\theta = t/\sigma^2$.

To obtain the norm bound (D.23), recall that $||Y||_2 = \max(\lambda_{\max}(Y), -\lambda_{\min}(Y))$. Standard Gaussian variables and Rademacher variables are symmetric, so the inequality above implies

$$\mathbb{P}\left(-\lambda_{\min}\left(\sum_k \xi_k A_k\right) \geq t\right) = \mathbb{P}\left(\lambda_{\max}\left(\sum_k (-\xi_k) A_k\right) \geq t\right) \leq d \cdot e^{-t^2/2\sigma^2}$$

Apply the union bound we have

$$\mathbb{P}\left(\left|\left|\sum_k \gamma_k A_k\right|\right|_2 \geq t\right) \leq \mathbb{P}\left(-\lambda_{\min}\left(\sum_k \xi_k A_k\right) \geq t\right) + \mathbb{P}\left(\lambda_{\max}\left(\sum_k (-\xi_k) A_k\right) \geq t\right) \leq 2d \cdot e^{-t^2/2\sigma^2}$$

□

D.4 Matrix Bennett and Bernstein Bounds

In the scalar setting, Bennett and Bernstein inequalities describe the upper tail of a sum of independent, zero-mean random variables that are either bounded or subexponential. In the matrix case, the analogous results concern a sum of zero-mean random matrices.

Lemma D.8 (Bounded Bernstein MGF)**.** Suppose that X is a random Hermitian matrix that satisfies

$$\mathbb{E}[X] = 0 \quad \text{and} \quad \lambda_{\max}(X) \leq 1 \quad \text{a.s.}$$

Then we have, for $\theta > 0$,

$$\mathbb{E}e^{\theta X} \preceq e^{\left(e^\theta - \theta - 1\right) \cdot \mathbb{E}[X^2]}$$

Proof of Lemma D.8. Fix the parameter $\theta > 0$, and define a smooth function f on the real line:

$$f(x) = \frac{e^{\theta x} - \theta x - 1}{x^2}$$

for $x \neq 0$ and $f(0) = \theta^2/2$. An exercise in differential calculus verifies that f is increasing. Therefore, $f(x) \leq f(1)$ when $x \leq 1$. The eigenvalues of X do not exceed one, so the transfer rule (D.2) implies that

$$f(X) \preceq f(I) = f(1) \cdot I$$

Expanding the matrix exponential and applying the latter relation, we discover that

$$e^{\theta X} = I + \theta X + X \cdot f(X) \cdot X$$

To complete the proof, we take the expectation of this semidefinite bound:

$$\mathbb{E}e^{\theta X} \preceq I + f(1) \cdot \mathbb{E}[X^2] \preceq \exp\left(f(1) \cdot \mathbb{E}[X^2]\right) = \exp\left(\left(e^\theta - \theta - 1\right) \cdot \mathbb{E}[X^2]\right)$$

The second semidefinite relation follows from (D.4). □

Theorem D.9 (Matrix Bernstein - Bounded Case)**.** Consider a finite sequence $\{X_k\}$ of independent, random, Hermitian matrices with dimension d. Assume that

$$\mathbb{E}[X_k] = 0 \quad \text{and} \quad \lambda_{\max}(X_k) \leq R \quad \text{a.s.}$$

Compute the norm of the total variance,

$$\sigma^2 := \left\| \sum_k \mathbb{E}[X_k^2] \right\|_2$$

Then the following chain of inequalities holds for all $t \geq 0$:

$$\begin{aligned} \mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) &\leq d \cdot \exp\left(-\frac{\sigma^2}{R^2} \cdot h\left(\frac{Rt}{\sigma^2}\right)\right) \quad \text{(Bennett inequality)} \\ &\leq d \cdot \exp\left(-\frac{t^2/2}{\sigma^2 + Rt/3}\right) \quad \text{(Bernstein inequality)} \\ &\leq \begin{cases} d \cdot \exp(-3t^2/8\sigma^2), & \text{for } t \leq \sigma^2/R \\ d \cdot \exp(-3t/8R), & \text{for } t \geq \sigma^2/R \end{cases} \quad \text{(split Bernstein inequality)} \end{aligned} \tag{D.25}$$

The function $h(u) := (1+u)\log(1+u) - u$ for $u \geq 0$.

Proof of Theorem D.9. We assume that $R = 1$; the general result follows by a scaling argument once we note that the summands are 1-homogeneous and the variance σ^2 is 2-homogeneous.

The main challenge is to establish the Bennett inequality, part (i); the ramining bounds are consequences of simple numerical estimates. Invoke Lemma D.8 to see that

$$\mathbb{E}[e^{\theta X_k}] \preceq e^{g(\theta)\cdot\mathbb{E}[X_k^2]}$$

where $g(\theta) := e^\theta - \theta - 1$ for $\theta > 0$. For each $\theta > 0$, Corollary D.5 implies that

$$\begin{aligned} \mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) &\leq d \cdot \exp\left(-\theta t + g(\theta) \cdot \lambda_{\max}\left(\sum_k \mathbb{E}[X_k^2]\right)\right) \\ &= d \cdot \exp\left(-\theta + g(\theta) \cdot \sigma^2\right) \end{aligned}$$

The right-hand side attains its minimal value when $\theta = \log(1 + t/\sigma^2)$. Substitute and simplify this value yields

$$-\theta t + g(\theta \cdot \sigma^2) = \sigma^2 \left(\frac{t}{\sigma^2} - \left(1 + \frac{t}{\sigma^2}\right)\log\left(1 + \frac{t}{\sigma^2}\right)\right) = -\sigma^2 h\left(\frac{t}{\sigma^2}\right)$$

where $h(u) := (1+u)\log(1+u) - u$ for $u \geq 0$, which leads to the result in establish part (i)

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq d \cdot \exp\left(-\sigma^2 h\left(\frac{t}{\sigma^2}\right)\right)$$

The Bennett inequality (i) implies the Bernstein inequality (ii) because of the numerical bound

$$h(u) \geq \frac{u^2/2}{1 + u/3} \quad \text{for} \quad u \geq 0$$

The latter relation is established by comparing derivatives. The Bernstein inequality (ii) implies the split

Bernstein inequality (iii). To obtain the sub-Gaussian piece of (iii), observe that

$$\frac{1}{\sigma^2 + Rt/3} \geq \frac{1}{\sigma^2 + R(\sigma^2/R)/3} = \frac{3}{4\sigma^2} \quad \text{for} \quad t \leq \sigma^2/R$$

becasue the left-hand side is a decreasing function of t for $t \geq 0$. Similarily, we obatin the subexponential piece of (iii) from the fact that

$$\frac{t}{\sigma^2 + Rt/3} \geq \frac{\sigma^2/R}{\sigma^2 + R(\sigma^2/R)3} = \frac{3}{4R} \quad \text{and} \quad t \geq \sigma^2/R$$

which holds because the left-hand side is an increasing function of t for $t \geq 0$. □

Theorem D.10 (Matrix Bernstein - Subexponential Case)**.** Consider a finite sequence $\{X_k\}$ of independent, random, Hermitian matrices with dimension d. Assume that

$$\mathbb{E}[X_k] = 0 \quad \text{and} \quad \mathbb{E}[X_k^p] \preceq \frac{p!}{2} \cdot R^{p-2} A_k^2$$

for $p = 2, 3, 4, \ldots$. Coompute the variance parameter $\sigma^2 := ||\sum_k A_k^2||_2$. Then the following chain of inequalities holds for all $t \geq 0$:

$$\begin{aligned} \mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) &\leq d \cdot \exp\left(-\frac{t^2/2}{\sigma^2 + Rt}\right) \\ &\leq \begin{cases} d \cdot \exp(-t^2/4\sigma^2) & \text{for } t \leq \sigma^2/R \\ d \cdot \exp(-t/4R) & \text{for } t \geq \sigma^2/R \end{cases} \end{aligned} \tag{D.26}$$

The hypotheses of Theorem D.10 are not fully comparable with the hypotheses of Theorem D.9, because Theorem D.10 allows the random matrices to be unbounded but it also demands that we control the fluctuation of the maximum and minimum eigenvalues.

D.5 Matrix Hoeffding and Azuma and McDiarmid

The scalar version of Azuma's inequality states that a scalar martingale exhibits normal concentration about its mean value, and the scale for deviations is controlled by the total maximum squared range of the difference sequence. Here is a matrix extension.

Lemma D.11 (Symmetrization)**.** Let H be a fixed Hermitian matrix, and let X bea random Hermitian matrix with $\mathbb{E}[X] = 0$. Then

$$\mathbb{E}\left[\operatorname{tr} e^{H+X}\right] \leq \mathbb{E}\left[\operatorname{tr} e^{H+2\sigma X}\right] \tag{D.27}$$

where σ is a Rademacher variable independent from X

Proof. Consturct an independent copy X' of the random matrix, and let $\mathbb{E}'$ denote integration with respect to the new variable. Since the matrix is zero mean,

$$\mathbb{E}\left[\operatorname{tr} e^{H+X}\right] = \mathbb{E}\left[\operatorname{tr}\ e^{H+X-\mathbb{E}'[X']}\right] \leq \mathbb{E}\left[\operatorname{tr}\ e^{H+(X-X')}\right] = \mathbb{E}\left[\operatorname{tr}\ e^{H+\sigma(X-X')}\right]$$

We have use the convexity of the trace exponential (both $\operatorname{tr}\exp(A)$ and $\operatorname{tr}\exp(-A)$ are convex) to justify the Jensen's inequality. Since $X - X'$ is a symmetric random matrix, we can modulate it by an independent Rademacher variable σ without changing its distribution. The final bound depends on a short sequence of inequalities:

$$\begin{aligned}
\mathbb{E}\left[\operatorname{tr} e^{H+X}\right] &\leq \mathbb{E}\operatorname{tr}\left(e^{H/2+\sigma X} \cdot e^{H/2-\sigma X'}\right) \quad \text{(Golden–Thompson (D.6))}\\
&\leq \mathbb{E}\left[\left(\operatorname{tr}\ e^{H+2\sigma X}\right)^{1/2} \cdot \left(\operatorname{tr}\ e^{H-2\sigma X}\right)^{1/2}\right] \quad \text{(Cauchy-Schwarz for the trace)}\\
&\leq \left(\mathbb{E}\left[\operatorname{tr}\ e^{H+2\sigma X}\right]\right)^{1/2} \cdot \left(\mathbb{E}\left[\operatorname{tr}\ e^{H+2\sigma X}\right]\right)^{1/2}\\
&= \mathbb{E}\left[\operatorname{tr}\ e^{H+2\sigma X}\right]
\end{aligned}$$

□

Lemma D.12 (Azuma CGF)**.** Suppose that X is a random Hermitian matrix and A is fixed Hermitian matrix satisfy $X^2 \preceq A^2$. Let σ be a Rademacher random variable independent from X. Then

$$\log \mathbb{E}\left[e^{2\sigma\theta X} \mid X\right] \preceq 2\theta^2 A^2 \quad \text{for} \quad \theta \in \mathbb{R}$$

Proof. We apply the Rademacher MGF bound, Lemma D.6, conditionally to obtain

$$\mathbb{E}\left[e^{2\theta\sigma X} \mid X\right] \preceq e^{2\theta^2 X^2}$$

The fact that the logarithm is operator monotone implies that

$$\log \mathbb{E}\left[e^{2\theta\sigma X} \mid X\right] \preceq 2\theta^2 X^2 \preceq 2\theta^2 A^2$$

where the second realtion follows from the hypothesis on X. □

Theorem D.13 (Matrix Azuma)**.** Consider a finite adpated sequence $\{X_k\}$ of Hermitian matrices in dimension d, and a fixed sequence $\{A_k\}$ of Hermitian matrices that satisfy

$$\mathbb{E}_{k-1}[X_k] = 0 \quad \text{and} \quad X_k^2 \preceq A_k^2 \quad \text{a.e.}$$

Compute the variance parameter

$$\sigma^2 := \left\|\sum_k A_k^2\right\|_2 = \lambda_{\max}\left(\sum_k A_k^2\right)$$

Then, for all $t \geq 0$,

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq d \cdot e^{-t^2/8\sigma^2} \tag{D.28}$$

Proof. The matrix Laplace transform method, Proposition D.1, states that

$$\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) \leq \inf_{\theta>0}\left\{e^{-\theta t} \cdot \mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right]\right\}$$

The main difficulty in the proof is to bound the matrix MGF, which we accomplish by an iterative argument that alternates between symmetrization and cumulant bounds.

Let us detail the first step of the iteration. Define the natural filtration $\mathcal{F}_k := \mathcal{F}(X_1, \dots, X_k)$ of the process $\{X_k\}$. Then we may compute

$$\begin{aligned}
\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right] &= \mathbb{E}\left[\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_{k=1}^{n-1}\theta X_k + \theta X_n\right)\middle|\mathcal{F}_{n-1}\right]\right] && \text{(iterated law)}\\
&\leq \mathbb{E}\left[\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_{k=1}^{n}\theta X_k + 2\sigma\theta X_n\right)\middle|\mathcal{F}_{n}\right]\right] && \text{(symmetrization)}\\
&\leq \mathbb{E}\left[\operatorname{tr}\exp\left(\sum_{k=1}^{n-1}\theta X_k + \log\mathbb{E}[e^{2\sigma\theta X_n} \mid \mathcal{F}_n]\right)\right] && \text{(concavity of trace exponential)}\\
&\leq \mathbb{E}\left[\operatorname{tr}\exp\left(\sum_{k=1}^{n-1}\theta X_k + 2\theta^2 A_n^2\right)\right] && \text{(Azuma CGF)}
\end{aligned}$$

- the first identity is the tower property of the conditional expectation
- in the second line, we winvoke the symmetrization method, Lemma D.11, conditional on $\mathcal{F}_{n-1}$, and then we relax the conditioning on the inner expectation to the larger algebra $\mathcal{F}_n$
- by construction, the Rademacher variable σ is independent from $\mathcal{F}_n$, so we can appy the concavity result, Corollary D.2, conditional on $\mathcal{F}_n$
- finally we use the fact (D.5) that trace exponential is monotone to introduce the Azuma CGF bound, Lemma D.12, in the last inequality

By iteration, we achieve

$$\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right] \leq \operatorname{tr}\exp\left(2\theta^2\sum_k A_k^2\right)$$

Note that this procedure relies on the fact that the sequence $\{A_k\}$ of upper bounds does not depend on the values of the random sequence $\{X_k\}$. Substitute the MGF bound into the Laplace transform bound above, and observe that the infimum is achieved when $\theta = t/4\sigma^2$, we have

$$\begin{aligned}
\mathbb{P}\left(\lambda_{\max}\left(\sum_k X_k\right) \geq t\right) &\leq \inf_{\theta>0}\left\{e^{-\theta t}\cdot\mathbb{E}\left[\operatorname{tr}\exp\left(\sum_k \theta X_k\right)\right]\right\}\\
&\leq \inf_{\theta>0}\left\{e^{-\theta t}\cdot\operatorname{tr}\exp\left(2\theta^2\sum_k A_k^2\right)\right\}\\
&\leq \inf_{\theta>0}\left\{e^{-\theta t}\cdot d\cdot\lambda_{\max}\left(\exp\left(2\theta^2\sum_k A_k^2\right)\right)\right\}\\
&= d\cdot\inf_{\theta>0}\left\{e^{-\theta t}e^{2\theta^2\sigma^2}\right\}\\
&= d\cdot e^{-\frac{t^2}{8\sigma^2}}
\end{aligned}$$

□