Introduction to Statistical Learning

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Session 3 - Mathematical tools: probability inequalities, complexity measures

Course overview

- Introduction

  Demystification / Learning and information / Setup

- Chapter 1 : Optimality in statistical learning

  Probabilistic view / Performance criteria / Optimal elements

- **Chapter 2 : Mathematical foundations of statistical learning**

  Concentration inequality / **Complexity measures** / Regularization

- Chapter 3 : Consistency of mainstream machine learning methods

  Boosting, SVM, Neural networks / Bagging, Random forests

Main messages of the Introduction

- Machine Learning is about **function estimation**
- Complexity of learning is closely related to compression in information theory : role of the "$\log K$" factor
- The key trade-off : **bias vs. variance**

Chapter 1 - Optimality in statistical learning

A. Modeling classification data : generative vs. discriminative
B. Optimality in the binary classification objective
C. Extensions of the plain classification problem
D. Convex risk minimization
E. Preference learning
F. The detection problem, ROC curve, AUC & co.

Main messages of Chapter 1

- To account for the uncertainty of evaluation, data are assumed to be sampled according to a *fixed* but *unknown* **probability distribution**.
- A prediction objective is characterized by an **error measure** and may be subject to **constraints**.
- The nature of **optimal elements** does tell something about the difficulty of the prediction objective.
- Convex risk minimization is relevant for classification thanks to **risk communication**
- Functional criteria like ROC or Precision-Recall curves are relevant in the context of **scoring and detection problems**

Chapter 2 - Mathematical tools

A. Probability inequalities
B. Complexity measures

————————exam material stops here !————————————

C. Regularization

Motivations

Statistical analysis of a generic principle known as Empirical Risk Minimization (ERM)

True error and empirical error

- Consider the binary classification prediction problem : $Y \in \{0, 1\}$
- Classifiers or predictors of the form : $h : \mathbb{R}^d \to \{0, 1\}$
- True error : $L(h) = \mathbb{P}\{Y \neq h(X)\}$
- Given a sample $D_n = \{(X_i, Y_i) : i = 1, \ldots, n\}$, the empirical error of h is defined as :

$$\widehat{L}_n(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{Y_i \neq h(X_i)\}$$

- Denote by $\mathcal{H}$ the class of candidate classifiers considered

Empirical risk minimization (ERM)

- Set the ERM classifier as :

$$\widehat{h}_n = \arg\min_{h \in \mathcal{H}} \widehat{L}_n(h)$$

- Define the best classifier in the class as :

$$\overline{h} = \arg\min_{h \in \mathcal{H}} L(h)$$

- We have :

$$L(\widehat{h}_n) - L(\overline{h}) \leq 2 \sup_{h \in \mathcal{H}} |L(h) - \widehat{L}_n(h)|$$

$\Rightarrow$ Need for uniform rates of convergence in the law of large numbers

Recall the key trade-off

- Denote by $L(h)$ the error measure for any decision function h
- Consider $\mathcal{H}$ the hypothesis space of decision functions
- We have : $L(\bar{h}) = \inf_{\mathcal{H}} L$, and $L(h^*) = \inf L$
- **Bias-Variance** type decomposition of error for any output $\widehat{h}$:

$$L(\widehat{h}) - L(h^*) = \underbrace{L(\widehat{h}) - L(\bar{h})}_{\text{estimation (stochastic)}} + \underbrace{L(\bar{h}) - L(h^*)}_{\text{approximation (deterministic)}}$$

Finite case (the "$\log K$")

Proposition (Uniform bound for finite classes)

Consider a finite family $\mathcal{H}$ of classifiers. We have, for any $\delta > 0$, with probability at least $1 - \delta$:

$$\forall h \in \mathcal{H} \ , \quad L(h) \leq \widehat{L}_n(h) + \sqrt{\frac{\log |\mathcal{H}| + \log\left(\frac{1}{\delta}\right)}{2n}}$$

Proof relies on : Hoeffding's inequality (see later) + union bound ($\mathbb{P}(A \cup B) \leq \mathbb{P}(A) + \mathbb{P}(B)$)

A. Probability inequalities

Key insight to concentration inequalities by Talagrand (1996) : "A random variable that depends (in a “smooth way”) on the influence of many independent variables (but not too much on any of them) is essentially constant."

Historical perspective

- Kolmogorov, Smirnov (1936) : convergence of empirical cdf to their expectations
- Dvoretsky, Kiefer, Wolfowitz (1956) : nonasymptotic version of Kolmogorov-Smirnov
- Hoeffding (1963) : deviation inequality (average of IID from its expectation
- Vapnik-Chervonenkis (1968) : equivalent of DKW for general measures (not only 1D on half lines)
- Mc Diarmid (1981) : first concentration inequality
- Massart (1990) : exact constant in DKW
- Talagrand (1996) : new concentration inequalities

Domains : uniform law of large numbers (and central limit theorem), empirical processes, large deviations, convex geometry, high dimensional probability

Reference : book by Boucheron-Lugosi-Massart (2013)

Hoeffding's lemma

Proposition

Consider Z a random variable such that :

- $\mathbb{E}(Z) = 0$
- $Z \in [a, b]$ *almost surely*

Then, for any $s > 0$, we have :

$$\mathbb{E}\left(e^{sZ}\right) \leq \exp\left(\frac{s^2(b-a)^2}{8}\right)$$

Interpretation : the Laplace transform of bounded random variables exhibits subgaussian behavior.

Hoeffding's inequality

Proposition

Consider $Z_1, \ldots, Z_n$ *IID over* $[0,1]$ *and* $\overline{Z}_n = \frac{1}{n}\sum_{i=1}^{n} Z_i$. *We then have, for any* $t > 0$

$$\mathbb{P}\{\overline{Z}_n - \mathbb{E}(Z_1) > t\} \leq \exp(-2nt^2)$$

and

$$\mathbb{P}\{\overline{Z}_n - \mathbb{E}(Z_1) < -t\} \leq \exp(-2nt^2)$$

Consequence : This bound implies the strong law of large numbers for bounded random variables (by Borel-Cantelli lemma)

Proof technique : Chernoff's bounding method

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} Z_i - \mathbb{E}(Z_1) > t\right) \leq \inf_{s>0} \exp\left(-nst + n\log\mathbb{E}(e^{s(Z_1 - \mathbb{E}(Z_1))})\right)$$

Beyond IID sequences

Definition. (Martingale difference)

Consider $V = (V_1, \ldots, V_n, \ldots)$ *and* $Z = (Z_1, \ldots, Z_n, \ldots)$ *two sequences of random variables. We call* V *a martingale difference sequence wrt* Z *if, for any* n *we have :*

- V_n *is a function of* $Z_1, \ldots, Z_n$
- $\mathbb{E}(V_{n+1} \mid Z_1, \ldots, Z_n) = 0$

A martingale inequality

Theorem. (Azuma's inequality)

Consider V a a martingale difference sequence wrt Z. Assume that, for any n, there exists U_n a function of $Z_1, \ldots, Z_{n-1}$ and $c_n \geq 0$ such that :

$$U_n \leq V_n \leq U_n + c_n$$

We then have, for any $t > 0$

$$\mathbb{P}\left(\sum_{i=1}^{n} V_i > t\right) \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^{n} c_i^2}\right)$$

and

$$\mathbb{P}\left(\sum_{i=1}^{n} V_i < -t\right) \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^{n} c_i^2}\right)$$

A basic concentration inequality

Theorem. (McDiarmid's inequality)

Consider $Z_1, \ldots, Z_n$ IID. Under a regularity assumption on the function f called the bounded difference assumption *with constant c/n, we have, for any $t > 0$*

$$\mathbb{P}\left(f(Z_1, \ldots, Z_n) - \mathbb{E}\big(f(Z_1, \ldots, Z_n)\big) > t\right) \leq \exp\left(-2nt^2/c^2\right)$$

and

$$\mathbb{P}\left(f(Z_1, \ldots, Z_n) - \mathbb{E}\big(f(Z_1, \ldots, Z_n)\big) < -t\right) \leq \exp\left(-2nt^2/c^2\right)$$

- Here the average of IID random variables is replaced by a general function of these IID variables.
- Take-home message : **Independence is more important/general than averaging**

Bounded difference assumption

- Consider a function f of n variables. We say that f has bounded differences if the variations along each variables are uniformly bounded.
- Here we need to have : for some $c > 0$

$$\sup_{z_1,\ldots,z_n,z_i'} |f(z_1,\ldots,z_n) - f(z_1,\ldots,z_{i-1},z_i',z_{i+1},\ldots,z_n)| \leq \frac{c}{n}$$

B. Complexity measures : From finite to infinite sets of functions

1. Metric complexities
2. Combinatorial complexities
3. Geometric complexities

Historical perspective

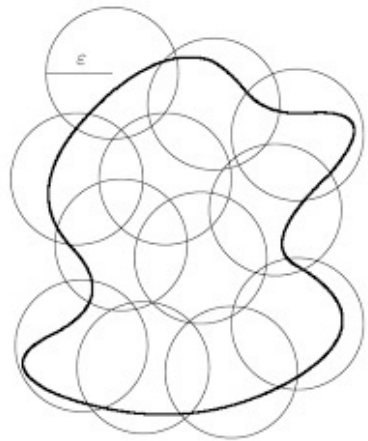
- Kolmogorov (1950's) : developed metric concepts such as covering numbers, metric entropy... in mathematical analysis.
- Vapnik and Chervonenkis (1970's) : discovered combinatorial concepts such as VC entropy, VC dimension and growth function in probability theory.
- Koltchinskii and Panchenko (2000) then Bartlett and Mendelson (2002) : baptized a geometry-related quantity Rademacher complexity which was a variation of gaussian complexity in the continuous case to solve some technical issues in machine learning theory.

B. Complexity measures

1. Complexity measures based on metric concepts (from dots to balls)

Covering numbers
Definition

- Consider a general space $\mathcal{H}$ (possibly space of functions) with a metric $\|\cdot\|$
- An ε-cover $\mathcal{T}$ is a set of elements of $\mathcal{H}$ such that for any $h \in \mathcal{H}$ there exists an element $t \in \mathcal{T}$ such that t is ε-close to h (i.e. $|h - t\| \leq \varepsilon$)



- The covering number $N(\varepsilon)$ is the cardinality of the smallest ε-cover of $\mathcal{H}$
- The metric entropy of $\mathcal{H}$ is the function $\varepsilon \mapsto \log N(\varepsilon)$

Covering numbers
Example

- Result : for the unit ball n $\mathbb{R}^d$, we have :

$$\left(\frac{1}{\varepsilon}\right)^d \leq N(\varepsilon) \leq \left(\frac{2}{\varepsilon} + 1\right)^d$$

Covering numbers
Upper bound on the error

Result by D. Pollard (1984)

- Notations : n sample size, ℓ loss function
- For bounded loss functions ($\|\ell(\cdot,\cdot)\| \leq M$), we have :

$$\mathbb{P}\left(\sup_{h\in\mathcal{H}} |L(h) - \hat{L}_n(h)| > \varepsilon\right) \leq N\left(\frac{\varepsilon}{8M}\right) \exp\left(-\frac{n\varepsilon^2}{2M^2}\right)$$

- Not easy to invert wrt to ε to obtain a clean error bound for $L(\hat{h}_n) - \inf_{h\in\mathcal{H}} L(h)$ (the variance part of the variance-bias for ERM)...

B. Complexity measures

2. Complexity concepts based on combinatorics (counting)

Vapnik-Chervonenkis (VC) entropy

- For a given sample $(X_1, \ldots, X_n)$ and for a given +1/-1 classifier h, denote by $X_n(h)$ the +1/-1 (classification) vector :

$$X_n(h) = (h(X_1), \ldots, h(X_n))^T \in \{-1, 1\}^n$$

- For this sample $(X_1, \ldots, X_n)$, denote by $\hat{N}(\mathcal{H})$ the cardinality of such vectors ("**colorings of the data**") induced by the set of functions $h \in \mathcal{H}$ (this set of vectors is sometimes called the *trace* of the set of functions on the sample). Note that there are at most 2^n vectors but can be less than 2^n since some vectors ("colorings') may be unreachable with functions in $\mathcal{H}$.

- VC entropy :

$$\mathcal{E}(\mathcal{H}) = \mathbb{E}(\log \hat{N}(\mathcal{H}))$$

Sufficient condition for the estimation error to go to zero

- Finite case (reminder) : convergence to zero of the estimation error if

$$\frac{\log |\mathcal{H}|}{n} \to 0 \ , \quad n \to \infty$$

- Similar role for the VC entropy : convergence to zero of the estimation error if

$$\frac{\mathcal{E}(\mathcal{H})}{n} = \frac{\mathbb{E}(\log \hat{N}(\mathcal{H}))}{n} \to 0 \ , \quad n \to \infty$$

- Questions : are there weaker conditions ? Which sets of functions fulfill such a condition ? What are the rates of convergence ?

VC dimension
Definition

- The VC dimension is the largest integer such that there exists a sample of n points in $\mathbb{R}^d$ for which all its "colorings" (separations in +1/-1 classes) can be achieved by elements of $\mathcal{H}$, *i.e.*

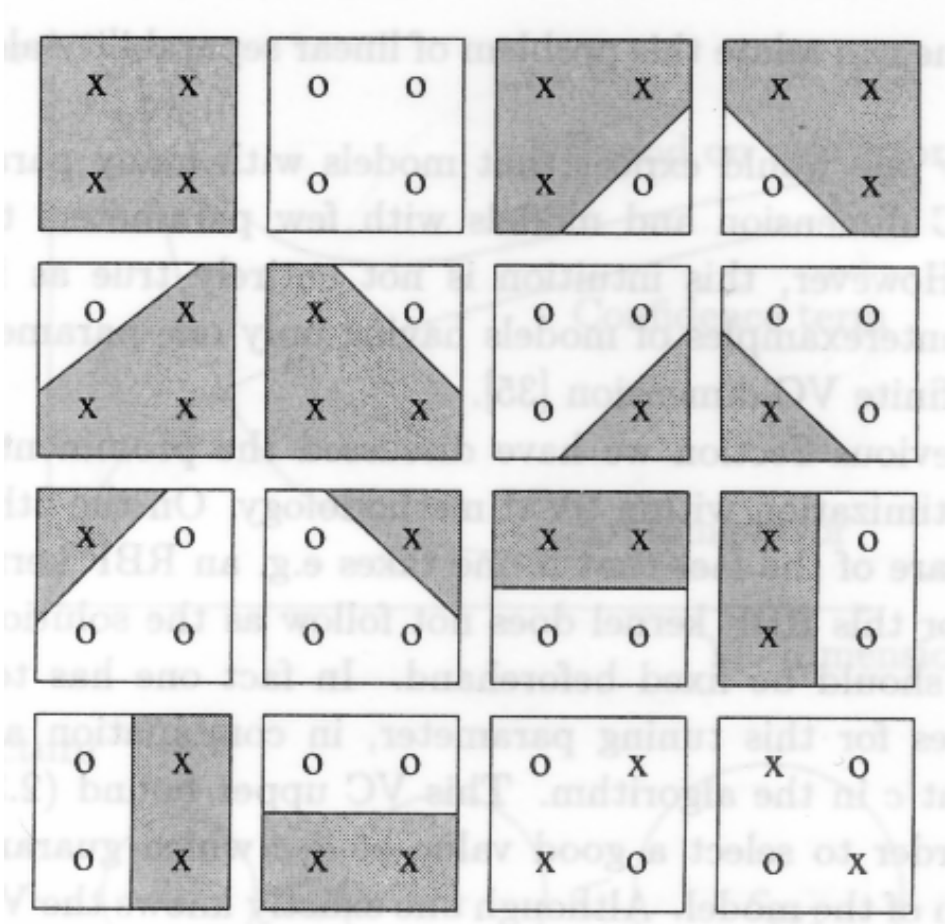
$$V(\mathcal{C}) = \max\{n \text{ integer } : \exists \text{ sample s.t.} |\hat{N}(\mathcal{H})| = 2^n\}$$

- By comparison to the VC entropy, the VC dimension corresponds to the "worst" sample since the expectation is replaced by a maximum over all possible training samples.

VC dimension
Examples

- Halfspaces in $\mathbb{R}^d$: $V = d + 1$
- Axis-aligned rectangles in $\mathbb{R}^2$: $V = 4$
- Just any rectangles in $\mathbb{R}^2$: $V = 7$
- Triangles in $\mathbb{R}^2$: $V = 7$
- Convex polygons in $\mathbb{R}^2$: $V = +\infty$

VC dimension
Halfplanes



Observation : Number of parameters is irrelevant

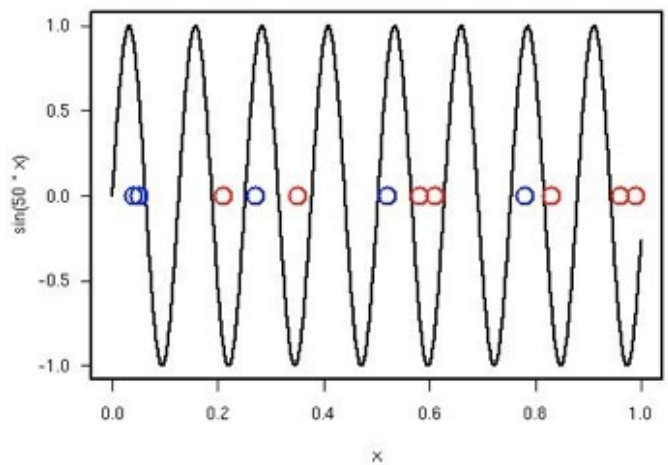
- Set of indicator functions parameterized by a single parameter ω :

$$h(x) = \mathbb{I}\{x : \sin(\omega x) > 0\} \ , \ \text{where } \omega \in [0, 2\pi)$$

- VC dimension of this set is infinite, using :

$$\omega = \frac{1}{2}\left(1 + \sum_{i=1}^{n}\left(\frac{1 - y_i}{2}\right)10^i\right)$$

for a set of points $x_j = 2\pi 10^{-j}$



Application : VC bound on classification error

- Assume $\mathcal{H}$ has finite VC dimension V. Then, we have, for any δ, with probability at least $1-\delta$:

$$L(\hat{h}_n) \leq \inf_{h \in \mathcal{H}} L(h) + \sqrt{\frac{2V \log\left(\frac{en}{V}\right)}{n}} + \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2n}}$$

- Behavior of the bound wrt V : as VC dimension V increases, the estimation error increases, but at the same time, it is expected that the approximation error goes down since the hypothesis space gets larger.

B. Complexity measures

3. Rademacher complexity : the modern approach to complexity

Learning Theory : Pre vs Post 2000

- Combinatorial complexity concepts (like VC-Dimension) were leading to loose bounds and raised technical difficulties. Cucker and Smale (2001) ; Evgeniou et al. (1999 ; 2000) ; Bartlett et al (1998) resolved various issues.
- Those complexity concepts also accounted for worst-case situations in terms of sample configuration. There was a challenge to develop data-dependent complexity measures (although it was possible).
- Two new approaches started in the late 1990s / early 2000s : **Stability** and **Rademacher complexity**.

Rademacher complexity
Why another concept ?

- The concept was already there in 1968 (Vapnik-Chervonenkis paper) but was not identified as a key quantity except used in an intermediate step of a proof which had to be simplified in later stages of the proof.

- It was rediscovered in 2000 by Koltchinskii and Panchenko and led to neater bounds and theory to encompass all state-of-the-art methods such as SVM, boosting and bagging, as well as neural nets.

A data-dependent view on complexity

- VC entropy is about counting ("coloring") vectors *on average wrt the training data* in the hypercube of $\mathbb{R}^n$ defined by vectors of the form :

$$X_n(h) = (h(X_1), \ldots, h(X_n))^T \in \{-1, 1\}^n \ , \qquad \text{for all } h \in \mathcal{H}$$

- Rademacher complexity is about estimating the average of the maximal correlation between a random binary-valued vector and the classification vector for a **fixed** training data set over the class of candidate classifiers.

Definition of Rademacher complexity

- Consider a sample of $D_n = (X_1, \ldots, X_n)$ of IID random variables, and a vector of Rademacher random variables : $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^T$ with ε_i's IID and independent of the training data such that $\mathbb{P}(\varepsilon_i = 1) = \mathbb{P}(\varepsilon_i = -1) = 1/2$
- Then the Rademacher complexity of the set of functions $\mathcal{H}$ is the sample-dependent quantity :

$$\hat{R}_n(\mathcal{H}) = \mathbb{E}\left(\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \varepsilon_i h(X_i) \middle| D_n \right) = \frac{1}{n} \mathbb{E}\left(\sup_{h \in \mathcal{H}} (\varepsilon^T X_n(h)) \middle| D_n \right)$$

Exercise : Rademacher complexity for linear classes

- Consider a sample $x_1, \ldots, x_n$ which are all contained in a ball with radius R
- Denote by $\mathcal{H}$ the hypothesis space of linear functions such that $h(x) = \beta^T x$ where $\|\beta\|_2 \leq M$
- We then have :

$$\hat{R}_n(\mathcal{H}) \leq \frac{MR}{\sqrt{n}}$$

Exercise : concentration of Rademacher complexity

- Set

$$f(X_1, \ldots, X_n) = \hat{R}_n(\mathcal{H}) = \mathbb{E}\left(\sup_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \varepsilon_i h(X_i) \middle| D_n \right)$$

- The function f satisfies the bounded differences assumption (why ?)
- Therefore, we have, by McDiarmid's inequality, with probability at least $1 - \delta$:

$$\mathbb{E}(\hat{R}_n(\mathcal{H}) \leq \hat{R}_n(\mathcal{H}) + \sqrt{\frac{\log(1/\delta)}{2n}}$$

Application to ERM

Theorem.

Expected error of ERM Let $\mathcal{H}$ be a class of classifiers from $\mathbb{R}^d$ to $\{-1, +1\}$

Consider $\widehat{h}_n$ the ERM classifier :

$$\widehat{h}_n = \arg\min_{h \in \mathcal{H}} \widehat{L}_n(h)$$

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

$$L(\widehat{h}_n) \leq \inf_{h \in \mathcal{H}} L(g) + \mathbb{E}(\widehat{R}_n(\mathcal{H}) + \sqrt{\frac{\log(1/\delta)}{2n}}$$

and

$$L(\widehat{h}_n) \leq \inf_{h \in \mathcal{H}} L(h) + \widehat{R}_n(\mathcal{H}) + 3\sqrt{\frac{\log(2/\delta)}{2n}}$$

Link between Rademacher complexity and VC dimension

- Rademacher bounded by VC dimension

$$\hat{R}_n(\mathcal{H}) \leq \sqrt{\frac{2\big(1+\log(n/V)\big)}{(n/V)}}$$

- This means that finite VC dimension implies that Rademacher complexity is of the order of $\sqrt{(\log n)/n}$
- However, there are classes with infinite VC dimension which have Rademacher complexity of the same order of magnitude $\sqrt{(\log n)/n}$

Coming next

- Next lectures :
  - Regularization and stability
  - Analysis of ML algorithms