Concentration of Measure for Machine Learning

An Introduction

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Outline

Motivation Missing Mass Estimation Binary Classification Learning Theory Dimensionality Reduction Chernoff's Method Basics Johnson-Lindenstrauss Lemma Non-parametric Bounds Extensions to dependent variables Negative association

KL Divergence and Lower Bounds Kullback-Leibler Divergence No Free Lunch Theorem Uniform Laws of Large Numbers Finite VC dimension implies Uniform Convergence Finite VC-dimension implies learnability



References

Cambridge Series in Statistical and Probabilistic Mathematics

High-Dimensional Statistics

A Non-Asymptotic Viewpoint

Martin J. Wainwright





CONCENTRATION INEQUALITIES



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Concentration Inequalities for the Missing Mass and for Histogram Rule Error

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Abstract

This paper gives distribution-free concentration inequalities for the minoing mass and the error rate of thiosegnen rules. A conject association for mobios can be used to reache these concentration probometry of the strength of the stre

1. Introduction

The Good-Turing missing mass estimator was developed in the 1940s to estimate the probability that the next item drawn from a fixed distribution will be an item net seen before. Since the publication of the Good-Turing missing mass estimator in 1953 (Good, 1953), this estimator has been used extensively in language modeling applications (Chen and Goodman, 1998, Church and Gale, 1991).





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Enigma



- Electro-mechanical rotor cipher machines, 26 characters
- Invented at the end of WW1 by Arthur Scherbius
- Commercial use, then German Army during WW2
- First cracked by Marian Rejewski in the 1930s (Bomb), then improved to $3.\,10^{114}$ configurations
- Read Simon Singh, The Code Book



Enigma



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Battle of the Atlantic



- Massively used by the German Kriegsmarine and Luftwaffe
- weakness: 3-letters setting to initiate communication, taken from the *Kenngruppenbuch*
- Government Code and Cypher School: Bletchley Park (on the train line between Cambridge and Oxford)
- Colossus (first programmable computers) in 1943





Estimating probabilities

- Discrete alphabet A.
- Unknown probability p on A
- Sample X_1, \ldots, X_n of independent draws of p.
- Goal : use the sample to estimate p(a) for all $a \in A$.

Natural idea:

$$\hat{p}(a) = \frac{N(a)}{n}$$
, where $N(a) = \#\{i : X_i = a\}$



Safari preparation









Bigram Model for NLP

Learning set: john read moby dick mary read a different book she read a book by cher

$$p(w_i|w_{i-1}) = \frac{c(w_{i-1}w_i)}{\sum_{w} c(w_{i-1}w)} \qquad p(s) = \prod_{i=1}^{l+1} p(w_i|w_{i-1})$$

p(john	read	а	book)
=	$p(\textit{john} \cdot)$	p(read john)	p(a read)	p(book a)	$p(\cdot \mathit{book})$
=	$\frac{c(\cdot \text{ john})}{\sum_{w} c(\cdot w)}$	$\frac{c(john \ read)}{\sum_{w} c(john \ w)}$	$\frac{c(reada)}{\sum_{w} c(read w)}$	$\frac{c(a \ book)}{\sum_{w} c(a \ w)}$	$\frac{c(book \cdot)}{\sum_{w} c(book w)}$
=	$\frac{1}{3}$	$\frac{1}{1}$	$\frac{2}{3}$	$\frac{1}{2}$	$\frac{1}{2}$
\approx	0.06				



Bigram Model for NLP

Learning set: john read moby dick mary read a different book she read a book by cher

$$p(w_i|w_{i-1}) = \frac{c(w_{i-1}w_i)}{\sum_{w} c(w_{i-1}w)} \qquad p(s) = \prod_{i=1}^{l+1} p(w_i|w_{i-1})$$



 \Rightarrow useless, the unseen **must** be treated correctly.



Bayesian Approach: Laplace Estimator

Pierre-Simon de Laplace (1749-1827), Thomas Bayes (1702-1761) Will the sun rise tomorrow?

 $\hat{\rho}(a) = \frac{N(a) + 1}{n + |A|}$

- good for small alphabets and many samples
- very bad when lots of items seen once (ex: DNA sequences)
- |A| can be very large (or even infinite), but *p* concentrated on few items
- \implies not a satisfying solution to the problem



Alan Turing

Irving J. Good



1912-1954 student of Godfrey Harold Hardy in Cambridge PhD from Princeton with Alonzo Church



1916-2009 Graduated in Cambridge Academic carrer in Bayesian statistics in Manchester and then in the University of Virginia (USA)





Missing mass estimation

 X_1, \ldots, X_n independent draws of $\rho \in \mathfrak{M}_1(A)$.

$$N_n(x) = \sum_{m=1}^n \mathbb{1}\{X_m = x\}$$



How to 'estimate' the total mass of the unseen items

$$M_n = \sum_{x \in A} p(x) \ \mathbb{1}\{N_n(x) = 0\} ?$$



Missing Mass

Let $A = \mathbb{N}$, let $p \in \mathcal{M}_1(\mathbb{N})$ and let $X_1, \ldots, X_n \stackrel{iid}{\sim} p$ and for every $x \in \mathbb{N}$, let $N_n(x) = \sum_{i=1}^n \mathbb{1}\{X_i = x\}$. Pb: estimate the mass of the unseen

$$M_n = \mathbb{P}(X_{n+1} \notin \{X_1, \dots, X_n\} | X_1^n) = \sum_{x=0}^{\infty} p(x) \mathbb{1}\{N_n(x) = 0\}$$

Idea: use *hapaxes* = symbols $x \in \mathbb{N}$ that appear once in the sample

$$\hat{M}_n = \frac{1}{n} \sum_{x=0}^{\infty} \mathbb{1}\left\{N_n(x) = 1\right\}$$

= Good-Turing 'estimator'

= *leave-one-out* estimator of M_n : if $X_{-i} = \{X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n\}$,

$$\hat{M}_n = \frac{1}{n} \sum_{i=1}^n \mathbb{1} \{ X_i \notin X_{-i} \}$$





'Bias' of the Good-Turing estimator

Proposition [Good '1953]

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Whatever the law *p*,

$$0 \leq \mathbb{E}\left[\hat{M}_{n}\right] - \mathbb{E}[M_{n}] \leq \frac{1}{n}$$
Proof:

$$\mathbb{E}\left[\hat{M}_{n}\right] - \mathbb{E}[M_{n}] = \frac{1}{n} \mathbb{E}\left[\sum_{x \in \mathbb{N}} \mathbb{1}\{N_{n}(x) = 1\}\right] - \mathbb{E}\left[\sum_{x \in \mathbb{N}} p(X)\mathbb{1}\{N_{n}(x) = 0\}\right]$$

$$= \frac{1}{n} \sum_{x \in \mathbb{N}} \mathbb{P}(N_{n}(x) = 1) - np(x) \mathbb{P}(N_{n}(x) = 0)$$

$$= \frac{1}{n} \sum_{x \in \mathbb{N}} np(x) (1 - p(x))^{n-1} - np(x) (1 - p(x))^{n}$$

$$= \frac{1}{n} \sum_{x \in \mathbb{N}} p(x) \times np(x) (1 - p(x))^{n-1}$$

$$= \frac{1}{n} \sum_{x \in \mathbb{N}} p(x) \mathbb{P}(N_{n}(x) = 1)$$

$$= \frac{1}{n} \mathbb{E}\left[\sum_{x \in \mathbb{N}} p(x)\mathbb{1}(N_{n}(x) = 1)\right] \in \left[0, \frac{1}{n}\right]$$

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Example: MNIST dataset









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Statistical Learning Hypothesis

Assumption

- The examples $(X_i, Y_i)_{1 \le i \le n}$ are iid samples of an unknown joint distribution \mathcal{D} ;
- The points to classify later are also independent draws of the same distribution $\mathcal{D}.$

Hence, for every *decision rule* $h:\mathcal{X}
ightarrow \mathcal{Y}$ we can define the *risk*

$$L_{\mathcal{D}}(h) = \mathbb{P}_{(X,Y)\sim\mathcal{D}}(h(X)\neq Y) = \mathcal{D}(\{(x,y):h(x)\neq y\}).$$

The goal of the learning algorithm is to *minimize the expected risk*:

$$R_n(\mathcal{A}_n) = \mathbb{E}_{\mathcal{D}^{\otimes n}}\left[L_{\mathcal{D}}\left(\underbrace{\mathcal{A}_n((X_1, Y_1), \dots, (X_n, Y_n))}_{\hat{h}_n}\right)\right]$$

for *every* distribution \mathcal{D} , using only the examples.



Binary Classification

- Domain $\mathcal X$, label space $\mathcal Y~=\{0,1\}$
- Unknown distribution <code>D</code> on $\mathcal{X} imes \mathcal{Y}$
- Sample $S = (X_1, Y_1), \dots, (X_n, Y_n) \stackrel{iid}{\sim} D$
- $h:\mathcal{X}
 ightarrow\mathcal{Y}$, $h\in\mathcal{H}$ hypothesis class
- loss function $\ell(y, y') = \mathbb{1}\{y \neq y'\}$
- generalization error (loss) $L_D(h) = \mathbb{E}_D[\ell(h(X), Y)] = \mathbb{E}_D[h(X) \neq Y]$

• training error
$$L_{S}(h) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\{h(X_{i}) \neq Y_{i}\}$$

- *agnostic* learning \neq realizable assumption (when there exists h^* such that $L_{\rm S}(h^*)=0$)
- learning algorithm: $S\mapsto \hat{h}_n$ such that $L_D(\hat{h}_n)-\inf_{h\in\mathcal{H}}L_D(h)$ small



Performance Limit: Bayes Classifier

Consider binary classification $\mathcal{Y} = \{0, 1\}$, $\eta(\mathbf{x}) := \mathcal{D}(\mathbf{Y} = 1 | \mathbf{X} = \mathbf{x})$.

Theorem

The Bayes classifier is defined by $h^*(x) = \mathbb{1}\{\eta(x) \ge 1/2\} = \mathbb{1}\{\eta(x) \ge 1 - \eta(x)\} = \mathbb{1}\{2\eta(x) - 1 \ge 0\}.$ For every classifier $h : \mathcal{X} \to \mathcal{Y} = \{0, 1\}$,

$$L_{\mathcal{D}}(h) \ge L_{\mathcal{D}}(h^*) = \mathbb{E}\Big[\min\big(\eta(X), 1 - \eta(X)\big)\Big].$$

The Bayes risk $L_D^* = L_D(h^*)$ is called the **noise** of the problem. More precisely,

$$\mathcal{L}_{\mathcal{D}}(h) - \mathcal{L}_{\mathcal{D}}(h^*) = \mathbb{E}\Big[\big| 2\eta(X) - 1 \big| \, \mathbb{1}\big\{ h(X) \neq h^*(X) \big\} \Big] \,.$$

Extends to $|\mathcal{Y}| > 2$.



Proof

$$\begin{split} L_{D}(h) - L_{D}(h^{*}) &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \Big(\\ &= \mathbb{1} \big\{ r = 1 \big\} \Big(\mathbb{1} \big\{ h^{*}(X) = 1 \big\} - \mathbb{1} \big\{ h^{*}(X) = 0 \big\} \big) \\ &+ \mathbb{1} \big\{ r = 0 \big\} \Big(\mathbb{1} \big\{ h^{*}(X) = 0 \big\} - \mathbb{1} \big\{ h^{*}(X) = 1 \big\} \big) \Big) \bigg] \\ &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \Big(2\mathbb{1} \big\{ r = 1 \big\} - 1 \Big) \Big(2\mathbb{1} \big\{ h^{*}(X) = 1 \big\} - 1 \Big) \bigg] \\ &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \Big(2\mathbb{1} \big\{ r = 1 \big\} - 1 \Big) \Big(2\mathbb{1} \big\{ \eta(X) \ge \frac{1}{2} \big\} - 1 \Big) \bigg] \\ &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \Big(2\mathbb{1} \big\{ \eta(X) \ge \frac{1}{2} \big\} - 1 \Big) \mathbb{E} \bigg[2\mathbb{1} \big\{ r = 1 \big\} - 1 \mid X \bigg] \bigg] \\ &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \Big(2\mathbb{1} \big\{ \eta(X) \ge \frac{1}{2} \big\} - 1 \Big) \Big(2\mathbb{E} \big[\mathbb{1} \big\{ r = 1 \big\} \mid X \big] - 1 \Big) \bigg] \\ &= \mathbb{E} \bigg[\mathbb{1} \big\{ h(X) \neq h^{*}(X) \big\} \sup \big(\eta(X) \ge \frac{1}{2} \big\} \big) \Big(2\eta(X) - 1 \big) \bigg] \end{split}$$



The Nearest-Neighbor Classifier

We assume that \mathcal{X} is a metric space with distance d. The nearest-neighbor classifier $\hat{h}_n^{NN} : \mathcal{X} \to \mathcal{Y}$ is defined as

$$\hat{h}_n^{NN}(x) = Y_l$$
 where $l \in \operatorname*{arg\,min}_{1 \leq i \leq n} d(x - X_i)$.

Typical distance: L^2 norm on \mathbb{R}^d : $||x - x'|| = \sqrt{\sum_{j=1}^d (x_i - x'_j)^2}$. Buts many other possibilities: Hamming distance on $\{0, 1\}^d$, etc.



Numerically







Numerically







The most simple analysis of the most simple algorithm

A1. $\mathcal{Y} = \{0, 1\}.$ A2. $\mathcal{X} = [0, 1[^d.$ A3. η is *c*-Lipschitz continuous:

$$\forall x, x' \in \mathcal{X}, \left|\eta(x) - \eta(x')\right| \le c ||x - x'||$$
.

Theorem

Under the previous assumptions, for all distributions ${\cal D}$ and all $m\geq 1$

$$\mathbb{E}\left[\mathcal{L}_{\mathcal{D}}\left(\hat{h}_{n}^{\mathsf{NN}}
ight)
ight]\leq 2\mathcal{L}_{\mathcal{D}}^{*}+rac{3c\sqrt{d}}{n^{1/(d+1)}}\;.$$



Proof Outline

- Conditioning: as $I(x) = \arg \min_{1 \le i \le n} ||x X_i||,$ $L_D(\hat{h}_n^{NN}) = \mathbb{E} \Big[\mathbb{E} \Big[\mathbb{1} \{ Y \ne Y_{I(X)} \} | X, X_1, \dots, X_n \Big] \Big].$ • $Y \sim \mathcal{B}(p), \ Y' \sim \mathcal{B}(q) \implies \mathbb{P}(Y \ne Y') \le 2 \min(p, 1 - p) + |p - q|,$ $\mathbb{E} \Big[\mathbb{1} \{ Y \ne Y_{I(X)} \} | X, X_1, \dots, X_n \Big] \le 2 \min(\eta(X), 1 - \eta(X)) + c ||X - X_{I(X)}||.$
- Partition \mathcal{X} into $|\mathcal{C}| = T^d$ cells of diameter \sqrt{d}/T :

$$\mathcal{C} = \left\{ \left[\frac{j_1 - 1}{\tau}, \frac{j_1}{\tau} \right] \times \cdots \times \left[\frac{j_d - 1}{\tau}, \frac{j_d}{\tau} \right], \quad 1 \leq j_1, \dots, j_d \leq \tau \right\} .$$

• 2 cases: either the cell of *X* is occupied by a sample point, or not:

$$\left\| X - X_{l(X)} \right\| \leq \sum_{c \in \mathcal{C}} \mathbb{1}\left\{ X \in c \right\} \left(\frac{\sqrt{d}}{T} \mathbb{1} \bigcup_{i=1}^{n} \left\{ X_{i} \in c \right\} + \sqrt{d} \mathbb{1} \bigcap_{i=1}^{n} \left\{ X_{i} \notin c \right\} \right) .$$

$$\mathbb{E}\left[\left\| X - X_{l(X)} \right\| \right] \leq \frac{\sqrt{d}}{T} + \frac{\sqrt{d}T^{d}}{en} \text{ and choose } T = \left\lfloor n^{\frac{1}{d+1}} \right\rfloor.$$

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What does the analysis say?

- Is it loose? (sanity check: uniform \mathcal{D}_{X})
- Non-asympototic (finite sample bound)
- The second term $\frac{3c\sqrt{d}}{n^{1/(d+1)}}$ is *distribution independent*
- Does not give the trajectorial decrease of risk
- In expectation only: concentrated?
- Exponential bound d (cannot be avoided...) \implies curse of dimensionality
- How to improve the classifier?



k-nearest neighbors

Let \mathcal{X} be a (pre-compact) metric space with distance d.

k-NN classifier

 $h^{k_{NN}}: x\mapsto \mathbbm{1}ig\{\hat{\eta}(x)\geq 1/2ig\}$ = plugin for Bayes classifier with estimator

$$\hat{\eta}(x) = \frac{1}{k} \sum_{j=1}^{k} Y_{(j)}(x)$$

where

$$d\big(X_{(1)}(X),X\big) \leq d\big(X_{(2)}(X),X\big) \leq \cdots \leq d\big(X_{(n)}(X),X\big) \ .$$
































Bias-Variance tradeoff

Risque de k-NN en fonction du nombre de voisins





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Agnostic PAC learnability

Definition

A hypothesis class \mathcal{H} is *agnostic PAC learnable* if there exists a function $n_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ and a learning algorithm $S \mapsto \hat{h}_n$ such that for every $\epsilon, \delta \in (0,1)$, for every distribution D on $\mathcal{X} \times \mathcal{Y}$ when $S = ((X_1, Y_1), \dots, (X_n, Y_n)) \stackrel{iid}{\sim} D$,

$$\mathbb{P}\Big(L_{D}(\hat{h}_{n}) \geq \inf_{h' \in \mathcal{H}} L_{D}(h') + \epsilon\Big) \leq \delta$$

for all $n \ge n_{\mathcal{H}}(\epsilon, \delta)$.

The smallest possible function $n_{\mathcal{H}}$ is called the *sample complexity* of learning \mathcal{H} .



Learning via uniform convergence

Definition

A training set *S* is called ϵ -representative (wrt domain $\mathcal{X} \times \mathcal{Y}$, hypothese class \mathcal{H} , loss function ℓ and distribution *D*) if

$$\forall h \in \mathcal{H}, \left| L_{S}(h) - L_{D}(h) \right| \leq \epsilon.$$

Lemma

If S is $\epsilon/2$ -representative, then any ERM \hat{h}_n defined by $\hat{h}_n \in \arg\min_{h \in \mathcal{H}} L_{\mathsf{S}}(h)$ satisfies:

$$L_D(\hat{h}_n) \leq \inf_{h \in \mathcal{H}} L_D(h) + \epsilon$$
.

Proof: for every $h \in \mathcal{H}$,

$$L_{D}(\hat{h}_{n}) \leq L_{S}(\hat{h}_{n}) + rac{\epsilon}{2} \leq L_{S}(h) + rac{\epsilon}{2} \leq L_{D}(h) + rac{\epsilon}{2} + rac{\epsilon}{2} \; .$$





Uniform Convergence Property

Definition

A hypothesis class \mathcal{H} has the *uniform convergence property* (wrt $\mathcal{X} \times \mathcal{Y}$ and ℓ) if there exists a function $n_{\mathcal{H}}^{UC} : (0,1)^2 \to \mathbb{N}$ such that for every $\epsilon, \delta \in (0,1)$ and for every distribution D over $\mathcal{X} \times \mathcal{Y}$, a sample $S = ((X_1, Y_1), \dots, (X_n, Y_n)) \stackrel{iid}{\sim} D$ of size $n \ge n_{\mathcal{H}}^{UC}(\epsilon, \delta)$ has probability at least $1 - \delta$ to be ϵ -representative.

Corollary

If \mathcal{H} has the uniform convergence property with a function $m_{\mathcal{H}}^{UC}$, then \mathcal{H} is agnostically PAC learnable with a sample complexity $n_{\mathcal{H}}(\epsilon, \delta) \leq n_{\mathcal{H}}^{UC}(\frac{\epsilon}{2}, \delta)$. Furthermore, the ERM is a successful PAC learner for \mathcal{H} .



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Dimensionality reduction

• Data:
$$X = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} \in \mathcal{M}_{n,p}(\mathbb{R}), p \gg 1.$$

- Dimensionality reduction: replace x_i with $y_i = Wx_i$, where $W \in \mathcal{M}_{d,p}(\mathbb{R})$, $d \ll p$.
- Hopefully, we do not loose too much by replacing x_i by y_i.
 2 approaches:
 - Quasi-invertibility: there exists a recovering matrix $U \in \mathcal{M}_{p,d}(\mathbb{R})$ such that for all $i \in \{1, \ldots, n\}$,

$$\tilde{x}_i = U y_i \approx x_i$$
.

- More modest goal: distance-preserving property

$$\forall 1 \leq i, j \leq n, \quad \|y_i - y_j\| \approx \|x_i - x_j\|$$



Johnson-Lindenstrauss Lemma

Theorem

Let $x_1, \ldots, x_n \in \mathbb{R}^p$, and let $\epsilon > 0$. Then, for every $d \ge \frac{4 \log(n)}{\epsilon - \log(1 + \epsilon)}$, there exists a matrix $A \in \mathcal{M}_{d,p}(\mathbb{R})$ such that

$$\forall 1 \leq i < j \leq n, \quad (1-\epsilon) \left\| x_i - x_j \right\|^2 \leq \left\| A x_i - A x_j \right\|^2 \leq (1+\epsilon) \left\| x_i - x_j \right\|^2.$$

d is independent of *p* (!) on the dependence on ϵ : $\frac{4\log(n)}{\epsilon - \log(1 + \epsilon)} \leq \frac{8\log(n)}{\epsilon^2} \left(1 + \frac{\epsilon}{3}\right)^2$.

Remark 2: how to find such a matrix *A***?** For every $d \ge \frac{4\log(n) + 2\log(1/\delta)}{\epsilon - \log(1 + \epsilon)}$, the probability that a *random matrix* with entries $A_{i,j} \stackrel{iid}{\sim} \mathcal{N}\left(0, \frac{1}{d}\right)$ satisfies the lemma is larger than $1 - \delta$.





Random Projections

Method: (constructive) probabilistic method: we choose

$$\mathsf{A}_{i,j} \stackrel{\textit{iid}}{\sim} \mathcal{N}\left(0, rac{1}{d}
ight) \;.$$

Let $y \in \mathbb{R}^{\rho}$ and Y = Ay. Then $\forall 1 \leq k \leq d$,

$$Y_k = \sum_{\ell=1}^{p} A_{k,\ell} y_\ell \sim \mathcal{N}\left(0, \frac{\|y\|^2}{d}\right) \;.$$

Hence $\mathbb{E}\left[\|\mathbf{Y}\|^2\right] = \|\mathbf{y}\|^2$.

 \implies does it hold with large probability?



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Classical Examples

- Gaussian
- Rademacher
- Bernoulli
- Poisson

Sub-Gaussian variables.



Chernoff's Bound

Theorem (Chernoff-Hoeffding Deviation Bound)

Let $\mu \in (0, 1)$. $X_1, \ldots, X_n \stackrel{iid}{\sim} \mathcal{B}(\mu)$, and let $x \in (\mu, 1]$.

(i) Chernoffs' bound for Bernoulli variables: $\mathbb{P}(\bar{X}_n \ge x) \le \exp(-n \operatorname{kl}(x, \mu))$, where

$$kl(\rho,q) = \rho \log \frac{p}{q} + (1-\rho) \log \frac{1-\rho}{1-q}$$
. Same for left deviations.

(ii) If $\phi(\mathbf{x}) = \mathrm{kl}(\mathbf{x},\mu)$, then $\phi^{\prime\prime}(\mathbf{x}) = 1/[\mathbf{x}(1-\mathbf{x})]$ and

$$\begin{split} \mathrm{d}(\mathbf{x},\mu) &= \frac{(\mathbf{x}-\mu)^2}{2} \int_0^1 \phi^{\prime\prime} \left(\mu + \mathbf{s}(\mathbf{x}-\mu)\right) \, 2(1-\mathbf{s}) \mathrm{d}\mathbf{s} \\ &\geq \frac{(\mathbf{x}-\mu)^2}{2\tilde{\mathbf{x}}(1-\tilde{\mathbf{x}})} \quad \text{with } \tilde{\mathbf{x}} = \frac{2\mu+\mathbf{x}}{3} \text{ by Jensen, since } \phi^{\prime\prime} \text{ is convex and } \int_0^1 \mathbf{s} \, 2(1-\mathbf{s}) \mathrm{d}\mathbf{s} = \frac{1}{3} \\ &\geq \frac{1}{2 \max_{\mathbf{x} \leq u \leq \mu} u(1-u)} \left(\mathbf{x}-\mu\right)^2 \quad \geq 2(\mathbf{x}-\mu)^2 \, . \end{split}$$

- (iii) Hoeffding's bound for Bernoulli variables: $\mathbb{P}(\bar{X}_n \ge x) \le \exp\left(-2n(x-\mu)^2\right)$.
- (iv) Inequalities (3) and (??) hold for arbitrary independent random variables with range [0, 1] and expectation μ . Reason: $\exp(\lambda x) \le (1 - x) \exp(0) + x \exp(\lambda)$.



k

Examples

 ${\boldsymbol{\cdot}} \ \, {\rm If} \, \mu < 1/2 {\rm ,} \\$

$$\mathbb{P}\left(\bar{X}_k > \frac{1}{2}\right) \le \exp\left(-\frac{k}{2}(1-2\mu)^2\right) \;.$$

(Consequence of Chernoff or direct computation with $(1-u)^k \leq exp(-ku)$, or of Hoeffding).

+ For all $\mu \in [0,1]$, Chernoff's bound with $\log(u) \geq (u-1)/u$ yields

$$\mathbb{P}\left(\bar{X}_m < \frac{\mu}{2}\right) \le \exp\left(-\frac{1 - \log(2)}{2} \, m\mu\right) \approx \exp\left(-0.153 \, m\mu\right) \le \exp\left(-\frac{m\mu}{7}\right)$$

Hoeffding yields a very poor result, but (ii) gives:

$$\mathbb{P}\left(\bar{X}_m < \frac{\mu}{2}\right) \le \exp\left(-\frac{3}{20}m\mu\right) = \exp\left(-0.15\,m\mu\right) \le \exp\left(-\frac{m\mu}{8}\right) \;.$$



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Proof of the Johnson-Lindenstrauss Lemma

Method: (constructive) probabilistic method: we choose $A_{i,j} \stackrel{iid}{\sim} \mathcal{N}\left(0, \frac{1}{d}\right)$. Let $y \in \mathbb{R}^{p}$ and

$$Y = Ay. \text{ Then } \forall 1 \le k \le d, Y_k = \sum_{\ell=1}^p A_{k,\ell} y_\ell \sim \mathcal{N}\left(0, \frac{\|y\|^2}{d}\right). \text{ Hence } \mathbb{E}\left[\|Y\|^2\right] = \|y\|^2.$$

Besides, by the deviation bound for the χ^2 distribution given in the next slide,

$$\mathbb{P}\left(\|\mathbf{Y}\|^2 \ge (1+\epsilon)\|\mathbf{y}\|^2\right) = \mathbb{P}\left(\sum_{k=1}^{a} \left(\frac{\sqrt{d}Y_k}{\|\mathbf{y}\|}\right)^2 \ge d(1+\epsilon)\right) \le \exp\left(-d\phi^*(\epsilon)\right) \le \frac{1}{n^2}$$

and similarly
$$\mathbb{P}\left(\left\|Y\right\|^2 \le (1-\epsilon)\left\|y\right\|^2\right) \le \exp\left(-d\phi^*(\epsilon)\right) \le \frac{1}{n^2}$$
.
Applying this result to all $y_{i,j} = x_i - x_j$, $1 \le i < j \le n$, by the union bound:

$$\mathbb{P}\bigg(\bigcup_{1\leq i< j\leq n} \left\|A(x_i-x_j)\right\| \geq (1+\epsilon) \cup \left\|A(x_i-x_j)\right\| \leq (1-\epsilon)\bigg) \leq \frac{n(n-1)}{n^2} < 1,$$

and hence there exists at least a matrix A for which the lemma holds.



Deviations of the χ^2 distribution: rate function

Lemma

If $\textit{U} \sim \mathcal{N}(0,1)$ and $\textit{X} = \textit{U}^2 - 1$, then

$$\phi^*(\mathbf{x}) = \sup_{\lambda} \lambda \mathbf{x} - \log \mathbb{E}\left[e^{\lambda \mathbf{x}}\right] = \frac{\mathbf{x} - \log(1 + \mathbf{x})}{2} \ge \frac{\mathbf{x}^2}{4\left(1 + \frac{\mathbf{x}}{3}\right)^2} \ .$$

Proof: For every $\lambda < 1/2$,

$$\mathbb{E}\left[e^{\lambda X}\right] = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{\lambda (u^2 - 1)} e^{-\frac{u^2}{2}} du = \frac{e^{-\lambda}}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-\frac{(1 - 2\lambda)u^2}{2}} du = e^{-\lambda} \frac{1}{\sqrt{1 - 2\lambda}} \ .$$

Hence $\phi(\lambda) = \log \mathbb{E}\left[e^{\lambda x}\right] = -\frac{1}{2}\log(1-2\lambda) - \lambda$. The concave function $\lambda \mapsto \lambda x - \phi(\lambda)$ is maximized at λ^* s.t. $x = \phi'(\lambda^*) = \frac{1}{1-2\lambda^*} - 1$, that is at $\lambda^* = \frac{1}{2}\left(1 - \frac{1}{1+x}\right) = \frac{x}{2(1+x)}$. Hence $\phi^*(x) = \lambda^* x - \phi(\lambda^*) = \frac{x - \log(1+x)}{2}$. The last inequality is obtained by "Pollard's trick" applied to $g(x) = x - \log(1+x)$: since g(0) = g'(0) = 0 and since $g''(x) = 1/(1+x)^2$ is convex, by Jensen's inequality

$$\frac{x - \log(1+x)}{x^{2}/2} = \int_{0}^{1} g''(sx)2(1-s)ds \ge g''\left(x \int_{0}^{1} s \ 2(1-s)ds\right) = g''\left(\frac{x}{3}\right)$$





Deviations of the $\chi^2(d)$ distribution

By Chernoffs method, if $Z \sim \chi^2(d) \stackrel{\text{dist}}{=} U_1^2 + \dots + U_d^2$ where $U_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$: $\mathbb{P}(Z \ge d(1+\epsilon)) \le \exp\left(-d\phi^*(\epsilon)\right) \le \exp\left(-\frac{d\epsilon^2}{4\left(1+\frac{\epsilon}{3}\right)^2}\right).$ Moreover, since $\phi^*(-\epsilon) = -\frac{\epsilon + \log(1-\epsilon)}{2} = \frac{1}{2}\sum_{k\ge 2} \frac{\epsilon^k}{k} \ge \frac{1}{2}\sum_{k\ge 2} (-1)^k \frac{\epsilon^k}{k} = \phi^*(\epsilon),$ $\mathbb{P}(Z \le d(1-\epsilon)) \le \exp(-d\phi^*(\epsilon)) \text{ and since } \phi^*(-\epsilon) = -\frac{\epsilon + \log(1-\epsilon)}{2} \ge \epsilon^2/4,$ $\mathbb{P}(Z \le d(1-\epsilon)) \le \exp\left(-\frac{2}{4}\right).$

Note: the Laurent-Massart inequality states that for every u > 0, $\mathbb{P}(\vec{z} \ge d + 2\sqrt{du} + 2u) \le \exp(-u)$. It can be deduced from the previous bound by noting that for every x > 0

$$\phi^* \left(2\sqrt{x} + 2x \right) = x + \frac{1}{2} \left(2\sqrt{x} - \log\left(1 + 2\sqrt{x} + \frac{\left(2\sqrt{x}\right)^2}{2}\right) \right)$$
$$\geq x + \frac{1}{2} \left(2\sqrt{x} - \log\left(\exp(2\sqrt{x})\right) \right) = x \text{, and}$$

 $\mathbb{P}\left(Z \ge d + 2\sqrt{du} + 2u\right) = \mathbb{P}\left(\frac{1}{d}\sum_{i=1}^{d} (U_i^2 - 1) \ge 2\sqrt{\frac{u}{d}} + 2\frac{u}{d}\right) \le \exp(-d\phi^*(2\sqrt{\frac{u}{d}} + 2\frac{u}{d})) \le e^{-u}.$ The proof of Laurent and Massart (which takes elements from Birgé and Massart 1998) is a bit different: they note that

$$\begin{split} \phi(\lambda) &= -\frac{1}{2}\log(1-2\lambda) - \lambda = \sum_{k=2}^{\infty} \frac{(2\lambda)^k}{2k} = \lambda^2 \sum_{\ell=0}^{\infty} \frac{4(2\lambda)^\ell}{2(\ell+2)} \le \lambda^2 \sum_{\ell=0}^{\infty} (2\lambda)^\ell = \frac{\lambda^2}{1-2\lambda}, \text{ and deduce that} \\ \phi^*(x) &\geq \psi^*(x) = \sup_{\lambda} \lambda x - \frac{\lambda^2}{1-2\lambda} = \frac{x+1-\sqrt{2x+1}}{2}, \text{ while } x > 0 \text{ and } \psi^*(x) = u \text{ implies } x = 2\sqrt{u} + 2u. \text{ Also note in passing that by } \\ \text{Pollard's trick } \phi^*(x) &\geq \psi^*(x) \ge \frac{x^2}{4\left(1+\frac{2x}{3}\right)^{3/2}}. \end{split}$$



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Bounded variables are sub-Gaussian

If $a \le X \le b$, then $\mathbb{V}ar[X] \le (b - a)^2/4$ By symmetrization, *X* is $(b - a)^2$ sub-Gaussian. In fact, one can prove better.



"Statistical Physics" View

Let *X* be a real-valued random variable with law P_X . For all $\lambda \in \mathbb{R}$, let $\phi_X(\lambda) = \ln \mathbb{E} \left[e^{\lambda X} \right]$. Then there is a largest open interval $[\lambda_{\min}, \lambda_{\max}]$ on which ϕ is defined. If it contains 0, let P_X^{λ} be defined by

$$\frac{dP_{\chi}^{\lambda}}{dP_{\chi}} = \frac{e^{\lambda\chi}}{\mathbb{E}\left[e^{\lambda\chi}\right]}$$

Then

$$\phi'(\lambda) = \mathbb{E}(\mathsf{P}_{\mathsf{X}}^{\lambda}) \quad and \quad \phi''(\lambda) = \mathbb{V}\!\mathrm{ar}(\mathsf{P}_{\mathsf{X}}^{\lambda})$$

Furthermore, let $(x_{\min}, x_{\max}) = [\lambda \mapsto \mathbb{E}(P_{\lambda})](\lambda_{\min}, \lambda_{\max})$, and let $\lambda(x)$ be it reciprocal mapping. Then for every $x > \mu := \mathbb{E}[X]$, $\mathbb{P}(Z > x) \le \exp(-I(x, \mu))$ and for every $x < \mathbb{E}[X]$, $\mathbb{P}(X < x) \le \exp(-I(x, \mu))$ where

$$I(x,\mu) = \sup_{\lambda_{\min} < \lambda < \lambda_{\max}} \lambda x - \phi_X(\lambda) .$$





Gibbs-Variance lemma

For any real-valued X with expectation $\mathbb{E}[X] = \mu$, any $x \in (x_{\min}, x_{\max})$ and $\lambda \in (\lambda_{\min}, \lambda_{\max})$,

$$\phi_{\mathsf{X}}(\lambda) = \lambda \mu + \int_0^\lambda \int_0^\lambda \sigma^2(t) \, dt \, du \; ,$$

and

$$\begin{split} l(x,\mu) &= \lambda(x)\beta(x) - \phi_X(\lambda(x)) \\ &= \mathrm{KL}\left(\mathsf{P}_{\beta(x)},\mathsf{P}_X\right) = \inf_{\mathbb{E}[Q] \ge x} \mathrm{KL}(Q,\mathsf{P}_X) \\ &= \int_{\mu}^{x} \int_{\mu}^{u} \frac{1}{\sigma^2(\lambda(t))} \, dt \, du \; . \end{split}$$



Chernoff's rate function and KL divergence

Let $P = P_{M_n}$ and for $\lambda \in \mathbb{R}$ let P_{λ} be defined by $\frac{dP_{\lambda}}{dP}(x) = \frac{e^{\lambda x}}{Z(\lambda)}$, ie for all measurable, non-negative function f: $\mathbb{E}_{\lambda}[f(X)] = \int_{\mathbb{R}} f(x) \frac{e^{\lambda x}}{Z(\lambda)} dP(x)$

Prop:

 $\begin{array}{l} \operatorname{KL}(\mathsf{P}_{\lambda},\mathsf{P}) = \lambda \mathbb{E}_{\lambda}[\mathsf{X}] - \Lambda(\lambda) = \inf \left\{ \operatorname{KL}(\mathsf{Q},\mathsf{P}) : \mathbb{E}_{\mathsf{Q}}[\mathsf{X}] \geq \mathbb{E}_{\lambda}[\mathsf{X}] \right\} \\ \text{Proof: For every } \mathsf{Q} \ll \mathsf{P} \text{ with } \mathbb{E}_{\mathsf{Q}}[\mathsf{X}] \geq \mathsf{x}, \end{array}$

$$KL(Q, P) = \int_{\mathbb{R}} \log\left(\frac{dQ}{dP}(x)\right) dQ(x)$$

$$= \int_{\mathbb{R}} \log\left(\frac{dQ}{dP_{\lambda}}(x)\frac{dP_{\lambda}}{dP}(x)\right) dQ(x)$$

$$= KL(Q, P_{\lambda}) + \int_{\mathbb{R}} \log\left(\frac{e^{\lambda x}}{Z(\lambda)}\right) dQ(x)$$

$$= KL(Q, P_{\lambda}) + \lambda \mathbb{E}_{Q}[X] - \log(Z(\lambda))$$

$$\geq 0 + \lambda \mathbb{E}_{\lambda}[X] - \Lambda(\lambda) = KL(P_{\lambda}, P)$$

Cor: since $\lambda(x)$ is such that $\mathbb{E}(P_{\lambda(x)}) = x$, $I(x) = KL(P_{\lambda(x)}, P)$



Chernoff's rate function and KL divergence

Let $P = P_{M_n}$ and for $\lambda \in \mathbb{R}$ let P_{λ} be defined by $\frac{dP_{\lambda}}{dP}(x) = \frac{e^{\lambda x}}{Z(\lambda)}$, ie for all measurable, non-negative function f: $\mathbb{E}_{\lambda}[f(X)] = \int_{\mathbb{R}} f(x) \frac{e^{\lambda x}}{Z(\lambda)} dP(x)$

Prop:

 $\mathrm{KL}(P_{\lambda}, P) = \lambda \mathbb{E}_{\lambda}[X] - \Lambda(\lambda) = \inf \left\{ \mathrm{KL}(Q, P) : \mathbb{E}_{Q}[X] \ge \mathbb{E}_{\lambda}[X] \right\}$ Cor: since $\lambda(x)$ is such that $\mathbb{E}(P_{\lambda(x)}) = x$, $I(x) = \overline{\mathrm{KL}}(P_{\lambda(x)}, P)$ Since $\Lambda'(\lambda) = \frac{\mathbb{E}\left[\chi e^{\lambda \chi}\right]}{\mathbb{E}\left[e^{\lambda \chi}\right]} = \mathbb{E}_{\lambda}[\chi]$ and $\Lambda''(\lambda) = \frac{\mathbb{E}\left[x^2 e^{\lambda X}\right]}{\mathbb{E}\left[e^{\lambda X}\right]} - \left(\frac{\mathbb{E}\left[X e^{\lambda X}\right]}{\mathbb{E}\left[e^{\lambda X}\right]}\right)^2 = \mathbb{V}\mathrm{ar}_{\lambda}[X] > 0, \text{ the } C^{\infty} \text{ mapping}$ $\lambda \mapsto \lambda x - \Lambda(\lambda)$ is maximal where at $\lambda(x)$ where $x = \Lambda'(\lambda(x)) = \mathbb{E}_{\lambda(x)}[X]$ and then $I(x) = \lambda(x)x - \Lambda(\lambda(x))$ $=\lambda(x)x - \left(\lambda(x)\mathbb{E}_{\lambda(x)}[X] - \mathrm{KL}\left(P_{\lambda(x)}, P\right)\right)$





Hoeffding's inequality

A [a, b]-bounded variable is $(b - a)^2/4$ -sub-Gaussian.



Application: Finite classes are agnostically PAC-learnable

Theorem

Let ${\cal H}$ be a finite hypothesis class. Then ${\cal H}$ enjoys the uniform convergence property with sample complexity

$$n_{\mathcal{H}}^{\mathcal{UC}}(\epsilon,\delta) \le \left\lceil \frac{\log \frac{2|\mathcal{H}|}{\delta}}{2\epsilon^2} \right\rceil$$

Moreover, $\mathcal H$ is agnostically PAC learnable using an ERM algorithm with sample complexity

$$n_{\mathcal{H}}(\epsilon, \delta) \leq 2n_{\mathcal{H}}^{\scriptscriptstyle UC}\left(rac{\epsilon}{2}, \delta
ight) \leq \left\lceil rac{2\lograc{2|\mathcal{H}|}{\delta}}{\epsilon^2}
ight
ceil$$

Proof: Hoeffding's inequality and the union bound.



Sub-Gaussian inequalities

Bennett's and Bernstein's inequalities

Let $(X_i)_{1 \le i \le n}$ be independent random variables upper-bounded by 1, let $\bar{\mu} = (\mathbb{E}[X_1] + \cdots + \mathbb{E}[X_n])/n$, let σ^2 be such that $\mathbb{E}[X_i^2] \le \sigma^2$ for all *i* and let $\phi(u) = (1+u)\log(1+u) - u$. Then, for all x > 0,

$$\mathbb{P}(\bar{x} \ge \bar{\mu} + x) \le \exp\left(-n\,\sigma^2\phi\left(\frac{x}{\sigma^2}\right)\right) \le \exp\left(-\frac{n\,x^2/2}{\sigma^2 + x/3}\right)$$

Bernstein from Bennett: $\phi(x) \ge \frac{x^2}{2(1+\frac{x}{3})}$ since $\psi(x) = 2(1+\frac{x}{3})\phi(x) - x^2 \ge 0$. Extension: if $X_i \le b$ with b > 0,

$$\mathbb{P}(\bar{X}_n \geq \bar{\mu} + x) \leq \exp\left(-\frac{n\sigma^2}{b^2}\phi\left(\frac{bx}{\sigma^2}\right)\right) \leq \exp\left(-\frac{nx^2/2}{\sigma^2 + bx/3}\right) .$$

Example: for X with range in [0, 1],

$$(\mu) \in \operatorname{cond}\left(-m\left(\frac{3}{2}\log\frac{3}{2}-\frac{1}{2}\right)\mu\right) \leq \exp\left(-\frac{3m\mu}{28}\right).$$
End by the lyon

Parenthesis: "Pollard's trick"

From [Pollard, MiniEmpirical ex.14, http://www.stat.yale.edu/-pollard/Books/Mini/Basic.pdf] For any sufficiently smooth real-valued function g defined at least in a neighborhood of 0 let

$$G(x) = rac{g(x) - g(0) - xg'(0)}{x^2/2} ext{ if } x
eq 0, ext{ and } G(0) = g''(0) \; .$$

By Taylor's integral formula $g(x) - g(0) - xg'(0) = \int_0^x g''(u)(x-u)du = x^2 \int_0^1 g''(sx)(1-s)ds$. Thus, $G(x) = \int g''(sx)d\nu(s)$, where $d\nu(s) = 2(1-s)\mathbbm{1}\{0 \le s \le 1\}ds$. Hence, if g is convex then $g'' \ge 0$ and $G \ge 0$. Moreover, if g'' is increasing then the functions $x \mapsto g''(sx)$ for $s \in [0, 1]$ are all increasing and G is also increasing as an average of increasing functions. For $g(u) = \exp(u)$, this yields that $(\exp(u) - u - 1)/u^2$ is increasing, as required for the proof of Bernstein's inequality. Similarly, if g'' is convex then G is also convex as an average of convex functions $(x \mapsto g''(sx))_s$. Moreover, by Jensen's inequality applied to convex function $\psi(s) = g''(xs)$ with the probability measure $d\nu(s) = 2(1-s)\mathbbm{1}\{0 \le s \le 1\}ds$.

$$G(x) = \int_0^1 g''(xs) \ 2(1-s)ds \ge g''\left(x \int_0^1 s \times 2(1-s)ds\right) = g''\left(\frac{x}{3}\right) \ .$$

For $\mathit{g}(\mathit{u}) = (1+\mathit{u})\log(1+\mathit{u}) - \mathit{u}, \mathit{g}''(\mathit{u}) = 1/(1+\mathit{u})$ and this yields:

$$\frac{g(u)}{u^2/2} \ge g''\left(\frac{u}{3}\right) = \frac{1}{1+u/3} \; .$$



Exercise: for $X_i \stackrel{iid}{\sim} \mathcal{B}(\mu)$, $\mathbb{P}(\bar{X}_m \ge 2\mu) \le \exp(-m \times ?)$

Chernoff + Taylor: since $\log(u) \ge (u - 1)/u$,

$$kl(2\mu,\mu) = 2\mu\log(2) + (1-2\mu)\log\frac{1-2\mu}{1-2\mu} \ge 2\mu\log(2) - \mu = \mu(2\log(2) - 1) \approx 0.386\,\mu \;.$$

Chernoff with convexity:

$$\operatorname{kl}(2\mu,\mu) \ge \frac{(2\mu-\mu)^2/2}{4/3\mu} = \frac{3}{8}\mu = 0.375\mu$$

Improved Hoeffding:

$$\mathrm{kl}(2\mu,\mu) \geq \frac{(2\mu-\mu)^2/2}{\max_{\mu \leq u \leq 2\mu} \mathit{u}(1-\mathit{u})} \geq \frac{\mu^2/2}{2\mu} = \frac{1}{4}\,\mu = 0.25\mu~.$$

Bennett:

$$2\mu \log \frac{2\mu}{\mu} - (2\mu - \mu) = \mu(2\log(2) - 1) \approx 0.386\,\mu \;.$$

Bernstein:

$$\frac{(2\mu-\mu)^2/2}{\mu(1-\mu)+(2\mu-\mu)/3} \ge \frac{\mu^2/2}{\mu+\mu/3}\frac{3}{8}\,\mu = 0.375\mu\;.$$

Hoeffding: $2(2\mu-\mu)^2=2\mu^2$, very poor (as expected) when μ is small.



Bennett's inequality

Theorem

Let $b \ge 0$ and let X be a centered variable such that $\mathbb{E}[X^2] \le \sigma^2$. If $\mathbb{P}(X \le b) = 1$, then for all $\lambda > 0$:

$$\mathbb{E}\left[e^{\lambda X}
ight] \leq \exp\left(rac{\sigma^2}{b^2}\left(e^{\lambda b}-\lambda b-1
ight)
ight) \;.$$

Hence, if $X = X_1 + \cdots + X_n$ where the (X_i) are independent, $X_i \le b$, $\mathbb{E}[X_i] = 0$ and $\mathbb{Var}[X_i] \le \sigma_i^2$, then for every x > 0,

$$\mathbb{P}(X > x) \le \exp\left(-\frac{\sigma^2}{b^2}H\left(\frac{bx}{\sigma^2}\right)\right)$$

with
$$\sigma^2 = \sum_{i=1}^n \sigma_i^2$$
.



Bernstein's inequality

Theorem If for all $k \ge 3$, $\mathbb{E}[X^k] \le 1/2k!\sigma^2 b^{k-2}$, then for all $\lambda \in (0, 1/b)$:

$$\mathbb{E}\left[\mathbf{e}^{\lambda\mathbf{X}}
ight] \leq \exp\left(rac{\lambda^2\sigma^2}{2(1-\lambda\mathbf{b})}
ight) \;.$$

Hence, if $X = X_1 + \cdots + X_n$ where the (X_i) are independent and $\forall k \geq 3$, $\mathbb{E}[X_i^k] \leq 1/2k!\sigma_i^2 b^{k-2}$, then for every x > 0,

$$\mathbb{P}(X > x) \le \exp\left(-\frac{x^2}{2\left(\sigma^2 + xb\right)}\right)$$

with $\sigma^2 = \sum_{i=1}^{n} \sigma_i^2$. Proof: choose $\lambda = x/(\sigma^2 + tb)$ Remark: Bennett's condition is stronger since it implies $\mathbb{E}[X^k] \le \mathbb{E}[X^2b^{k-2}] \le \sigma^2b^{k-2}$.



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Hoeffding-Azuma

Th: Let X_0, \ldots, X_n be a martingale such that $\forall 1 \le k \le n, |X_k - X_{k-1}| \le c_k$. Then for all x > 0,

$$\mathbb{P}(|X_n - X_0| > x) \le 2 \exp\left(-\frac{x^2}{2\sum_{k=1}^n c_k^2}\right)$$



Mc-Diarmid's ineqality

McDiarmid's inequality: If X_1, \ldots, X_n are independent random variables on \mathcal{X} and $f : \mathcal{X}^n \to \mathbb{R}$ is such that $\forall 1 \le i \le n, \forall x_1, \ldots, x_n, x'_i$,

$$f(x_1, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_n) - f(x_1, \ldots, x_{i-1}, x'_i, x_{i+1}, \ldots, x_n) \Big| \leq c_i$$

then

$$\mathbb{P}\Big(\Big|f(X_1,\ldots,X_n)-\mathbb{E}\big[f(X_1,\ldots,X_n)\big]\Big|\geq x\Big)\leq \exp\left(\frac{-2x^2}{\sum_{i=1}^n c_i^2}\right)\ .$$

Sanity check: $f(x) = \sum x_i$ Application to the concentration of the Good-Turing estimator.



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A first concentration result with Chebishev: negative correlation permits to bound the variance of M_n by 1/(en).



Teaser: Missing mass - negative correlation


References For Negative Association

Negative Association - Definition, Properties, and Applications, by David Wajc https://www.cs.cmu.edu/~dwajc/notes/Negative%20Association.pdf

Balls and Bins: A Study in Negative Dependence, by Balls and Bins: A Study in Negative Dependence, https://www.brics.dk/RS/96/25/BRICS-RS-96-25.pdf



Definition

Intuitively: X_1, \ldots, X_n are negatively associated when, if a subset *I* a variables is "high", a disjoint subset *J* has to be "low".

Definition

A set of real-valued random variables $X_1, X_2, ..., X_n$ is said to be negatively associated (NA) if for any two disjoint index sets $I, J \subset [n]$ and two functions f, g both monotone increasing or both monotone decreasing, it holds

$$\mathbb{E}\left[f(X_i:i\in I)\,g(X_j:j\in J)\right] \leq \mathbb{E}\left[f(X_i:i\in I)\right]\,\mathbb{E}\left[g(X_j:j\in J)\right]$$

NB: *f* is monotone increasing if $\forall i \in I, x_i \leq x'_i$ implies $f(x) \leq f(x')$.



First properties

Let $X_1, X_2, ..., X_n$ be NA.

- For all $i \neq j$, $\mathbb{E}[X_iX_j] \leq \mathbb{E}[X_i] \mathbb{E}[X_j]$ i.e. $\operatorname{Cov}(X_i, X_j) \leq 0$.
- For any disjoints subsets $I, J \subset [n]$ and all x_1, \ldots, x_n ,

 $\mathbb{P}(X_i \ge x_i : i \in I \cup J) \le \mathbb{P}(X_i \ge x_i : i \in I) \ \mathbb{P}(X_j \ge x_j : j \in J) \text{ and } \\ \mathbb{P}(X_i \le x_i : i \in I \cup J) \le \mathbb{P}(X_i \le x_i : i \in I) \ \mathbb{P}(X_j \le x_j : j \in J)$

• For all monotone increasing functions f_1, \ldots, f_k depending on disjoint subsets of the $(X_i)_{i_i}$

$$\mathbb{E}\Big[\prod_{j}f_{j}(X)\Big] \leq \prod_{j}\mathbb{E}\big[f_{j}(X)\big]$$

• For all *x*₁,...,*x*_n,

$$\mathbb{P}\left(\bigcap_{i} \left\{X_{i} \geq x_{i}\right\}\right) \leq \prod_{i} \mathbb{P}(X_{i} \geq x_{i}) \quad \text{and} \quad \mathbb{P}\left(\bigcap_{i} \left\{X_{i} \leq x_{i}\right\}\right) \leq \prod_{i} \mathbb{P}(X_{i} \leq x_{i})$$





Consequence: NA concentrates better than independent

For Chernoff's method (which relies on exponential moments), NA variables can simply be treated as independent! In particular:

Chernoff-Hoeffding bound

Let X_1, \ldots, X_n be NA random variables with $X_i \in [a_i, b_i]$ a.s. Then $S = X_1 + \cdots + X_n$ satifies Hoeffding's tail bound: for all $t \ge 0$,

$$\mathbb{P}\Big[\big|\mathsf{S}-\mathsf{E}[\mathsf{S}]\big| \ge t\Big] \le 2\exp\left(-\frac{2t^2}{\sum_i(b_i-a_i)^2}\right)$$



Examples of NA variables

- Independent variables...
- **0-1 principle** If X_1, \ldots, X_n are Bernoulli variables and $\sum_i X_i \le 1$ a.s., then they are NA.

Let *f* and *g* are monotically increasing and depend on disjoint subsets of indices. $\mathbb{E}[f(X)g(X)] \leq \mathbb{E}[f(X)] \mathbb{E}[g(X)] \iff \mathbb{E}[\tilde{f}(X)] \mathbb{E}[\tilde{g}(X)]$, where $\tilde{f}(X) = f(X) - f(\tilde{O})$ and $\tilde{g}(X) = g(X) - g(\tilde{O})$. But $\tilde{f}(X)\tilde{g}(X) = O$ always, while $\tilde{f}(X) \geq 0$ and $\tilde{g}(X) \geq 0$.

- **Permutation distributions** If $x_1 \leq \cdots \leq x_n$ and if X_1, \ldots, X_n are random variables such that $\{X_1, \ldots, X_n\} = \{x_1, \ldots, x_n\}$ a.s., with all assignments equally likely, then they are NA.
- Sampling without replacement If X_1, \ldots, X_n are sample without replacement from $\{x_1, \ldots, x_N\}$ (with $N \ge n$), then they are NA.



Closure properties

Union

If the $\{X_i : i \in I\}$ are NA, if $\{Y_j : j \in J\}$ are NA, and if the $\{X_i\}$ are independent from the $\{Y_j\}$, then the $\{X_i, Y_j : i \in I, j \in J\}$ are NA.

Concordant monotone

If the $\{X_i : i \in I\}$ are NA, if $f_1, \ldots, f_k : \mathbb{R}^n \to \mathbb{R}$ are all monotonically increasing and depend on different subsets of [n], then $\{f_j(X) : 1 \le j \le k\}$ are NA. The same holds if $f_1, \ldots, f_k : \mathbb{R}^n \to \mathbb{R}$ are all monotonically decreasing.



Bins and balls

The standard bins and balls process consists of *m* balls and *n* bins.

- each ball *b* is independently placed in bin *i* with probability $p_{b,i}$: $X_b \stackrel{indep}{\sim} \mathcal{M}ulti(p_{b,\cdot})$.
- occupancy number $B_i = \sum_{b=1}^m \mathbb{1}\{X_b = i\}$ number of balls in bin *i*.

In particular $\sum_{i=1}^{n} B_i = m$. **Prop:** The B_i are NA.

Let $X_{b,i} = 1$ { ball b fell into bin i}. By the 0 - 1 principle, for all $1 \le b \le m$ the { $X_{b,i} : 1 \le i \le n$ } are NA. By independence and dosure under union, so are the { $X_{b,i} : 1 \le b \le m, 1 \le i \le n$ }. By closure under concordant monotone functions, the $B_i = \sum_{b=1}^{m} X_{b,i}$ are NA.

Consequence: Concentration of the number $N = \sum_{i} \mathbb{1}\{B_{i} = 0\}$ of empty bins, since the $(\mathbb{1}\{B_{i} = 0\})_{i}$ are NA.

If $p_{b,i} = 1/n$, then the number N of empty bins satisfies $N = n e^{-m/n} \pm O(\sqrt{n e^{-m/n}})$.



Applications

- missing mass
- · histogram rules for binary classification



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Finite VC dimension implies Uniform Convergence

Finite VC_Tdimension implies learnability



Kullback-Leibler divergence

Definition

Let *P* and *Q* be two probability distributions on a measurable set Ω . The Kullback-Leibler divergence from *Q* to *P* is defined as follows:

- if *P* is not absolutely continuous with respect to *Q*, then $KL(P, Q) = +\infty$;
- otherwise, let $\frac{dP}{dQ}$ be the Radon-Nikodym derivative of P with respect to Q. Then

$$\mathrm{KL}(P,Q) = \int_{\Omega} \log \frac{dP}{dQ} \, dP = \int_{\Omega} \frac{dP}{dQ} \log \frac{dP}{dQ} \, dQ \; .$$

 $\begin{array}{l} \label{eq:property: 0} \underset{\ensuremath{\left|} P \mbox{ or } g \mbox{ of } g \mbox{$



Lower Bound: Change of Measure

For all $\epsilon > 0$ and all $\alpha > 0$,





Lower Bound: Change of Measure

For all $\epsilon > 0$ and all $\alpha > 0$,

Asymptotic Optimality (Large Deviation Lower Bound)

$$\liminf_{n} \frac{1}{n} \log \mathbb{P}_{\mu} (\bar{X}_n \ge x) \ge -\operatorname{kl}(x, \mu) .$$



Lower Bound: Change of Measure

For all $\epsilon > 0$ and all $\alpha > 0$,

$$\mathbb{P}_{\mu} \left(\bar{X}_{n} \geq x \right) = \mathbb{E}_{\mu} \left[\mathbb{1} \left\{ \bar{X}_{n} \geq x \right\} \right]$$

$$\geq \mathbb{E}_{x+\epsilon} \left[\mathbb{1} \left\{ \bar{X}_{n} \geq x \right\} \mathbb{1} \left\{ \frac{1}{n} \sum_{i=1}^{n} \log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{i}) \leq \mathbb{E}_{x+\epsilon} \left[\log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{1}) \right] \right]$$

$$\times e^{-\sum_{i=1}^{n} \log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{i})} \right]$$

$$\geq e^{-n \left\{ \mathbb{E}_{x+\epsilon} \left[\log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{1}) \right] + \alpha \right\}} \left[\mathbb{1} - \mathbb{P}_{x+\epsilon} \left(\bar{X}_{n} < x \right) - \mathbb{P}_{x+\epsilon} \left(\frac{1}{n} \sum_{i=1}^{n} \log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{i}) > \mathbb{E}_{x+\epsilon} \left[\log \frac{dP_{x+\epsilon}}{dP_{\mu}} (X_{1}) \right] + \alpha \right) \right]$$

$$= e^{-n \left\{ \mathbb{E}_{x+\epsilon}(x_{i}, x_{i}) + \alpha \right\}} (1 - o_{n}(1)) .$$

Asymptotic Optimality (Large Deviation Principle)

$$\frac{1}{n}\log \mathbb{P}_{\mu} (\bar{X}_n \geq x) \underset{n \to \infty}{\longrightarrow} - \mathrm{kl}(x, \mu) \ .$$



Properties of KL divergence Tensorization of entropy:

If $\textit{P} = \textit{P}_1 \otimes \textit{P}_2$ and $\textit{Q} = \textit{Q}_1 \otimes \textit{Q}_2$, then

 $\mathrm{KL}(\mathsf{P},\mathsf{Q}) = \mathrm{KL}(\mathsf{P}_1,\mathsf{Q}_1) + \mathrm{KL}(\mathsf{P}_2,\mathsf{Q}_2) \; .$

Contraction of entropy data-processing inequality:

Let (Ω, \mathcal{A}) be a measurable space, and let P and Q be two probability measures on (Ω, \mathcal{A}) . Let $X : \Omega \to (\mathcal{X}, \mathcal{B})$ be a random variable, and let P^X (resp. Q^X) be the push-forward measures, ie the laws of X wrt P (resp. Q). Then

 $\mathrm{KL}\left(P^{X},Q^{X}\right)\leq\mathrm{KL}(P,Q)$.

Pinsker's inequality:

Let $P, Q \in \mathfrak{M}_1(\Omega, \mathcal{A})$. Then $\|P - Q\|_{TV} \stackrel{\text{def}}{=} \sup_{A \in \mathcal{A}} |P(A) - Q(A)| \le \sqrt{\frac{\mathrm{KL}(P, Q)}{2}}$.



Proof: contraction

Contraction: if KL(P, Q) = $+\infty$, the result is obvious. Otherwise, $P \ll Q$ and there exists $\frac{dP}{dQ} : \Omega \to \mathbb{R}$ such that for all measurable $f : \Omega \to \mathbb{R}, \int_{\Omega} f dP = \int_{\Omega} f \frac{dP}{dQ} dQ$.

• We first prove that $P^X \ll Q^X$ and, if $\gamma(x) := \mathbb{E}_Q \begin{bmatrix} \frac{dP}{dQ} | X = x \end{bmatrix}$ is the Q-a.s. unique function such that $\mathbb{E}_Q \begin{bmatrix} \frac{dP}{dQ} | X \end{bmatrix} = \gamma(X)$, then $\gamma = \frac{dP^X}{dQ^X}$. Indeed, for all $B \in \mathcal{B}$,

$$P^{X}(B) = P(X \in B) = \int_{X \in B} \frac{dP}{dQ} dQ = \mathbb{E}_{Q} \left[\frac{dP}{dQ} \mathbb{1} \{ X \in B \} \right]$$
$$= \mathbb{E}_{Q} \left[\mathbb{E}_{Q} \left[\frac{dP}{dQ} \mathbb{1} \{ X \in B \} | X \right] \right] = \mathbb{E}_{Q} \left[\mathbb{1} \{ X \in B \} \mathbb{E}_{Q} \left[\frac{dP}{dQ} | X \right] \right]$$
$$= \mathbb{E}_{Q} \left[\mathbb{1} \{ X \in B \} \gamma(X) \right] = \int_{X \in B} \gamma(X) dQ = \int_{B} \gamma dQ^{X}$$

and hence $P^{\chi} \ll Q^{\chi}$ and $\frac{dP^{\chi}}{dQ^{\chi}}$ • Now, $VI \left(P^{\chi} - Q^{\chi} \right)$

$$\begin{aligned} \int_{\Omega} \operatorname{and} \frac{1}{dQ^{X}} &= \gamma. \\ \operatorname{KL} \left(P^{X}, Q^{X} \right) &= \int_{\mathcal{X}} \gamma \log \gamma \ dQ^{X} = \int_{\Omega} \gamma(X) \log \gamma(X) \ dQ \\ &= \mathbb{E}_{Q} \left[\phi \left(E_{Q} \left[\frac{dP}{dQ} \middle| X \right] \right) \right] \quad \text{where } \phi := x \mapsto x \log(x) \text{ is convex} \\ &\leq \mathbb{E}_{Q} \left[\mathbb{E}_{Q} \left[E_{Q} \left[\phi \left(\frac{dP}{dQ} \right) \middle| X \right] \right] \quad \text{by (conditional) Jensen's inequality} \\ &= \mathbb{E}_{Q} \left[\phi \left(\frac{dP}{dQ} \right) \right] = \operatorname{KL}(P, Q) . \end{aligned}$$





Proof: Pinsker

Let $A \in \mathcal{A}$, p = P(A) and q = Q(A). By contraction,

 $KL(P,Q) \geq KL(P^{\mathbb{1}_A},Q^{\mathbb{1}_A}) = KL\left(\mathcal{B}\big(P(A)\big),\mathcal{B}\big(Q(A)\big)\right) = kl\left(P(A),Q(A)\right) \geq 2\big(P(A)-Q(A)\big)^2 \ .$



Lower Bound: the Entropic Way



A non-asymptotic lower bound



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The No-Free-Lunch theorem

A learning algorithm *A* for binary classification maps a sample $S \sim D^{\otimes n}$ to a decision rule \hat{h}_n .

Theorem

Let A be any learning algorithm for binary classification over a domain \mathcal{X} . If the training set size is $n \leq |\mathcal{X}|/2$, then there exists a distribution \mathcal{D} over $\mathcal{X} \times \{0, 1\}$ such that:

- there exists a function $f: \mathcal{X} \to \{0, 1\}$ with $\mathcal{L}_{\mathcal{D}}(f) = 0$;
- with probability at least 1/7 over the choice of S $\sim \mathcal{D}^{\otimes n}$,

$$L_{\mathcal{D}}(A(S)) \geq \frac{1}{8}$$
.

Note that the ERM over $\mathcal{H} = \{f\}$, or over any set \mathcal{H} such that $n \ge 8\log(7|\mathcal{H}|/6)$, is a successful learner in that setting.



Proof

Take $C \subset \mathcal{X}$ of cardinality 2n, and $\{0, 1\}^C = \{f_1, \ldots, f_T\}$ where $T = 2^{2n}$. For each $1 \leq i \leq T$, we denote by D_i the probability distribution on $C \times \{0, 1\}$ defined by $D_i(\{x, y\}) = \begin{bmatrix} \frac{1}{2n} & \text{if } y = f_i(x) \\ 0 & \text{otherwise.} \end{bmatrix}$

We will show that $\max_{1 \le i \le T} \mathbb{E}[\iota_{D_j}(A(S))] \ge 1/4$, which entails the result thanks to the small lemma: if $P(0 \le Z \le 1) = 1$ and $\mathbb{E}[Z] \ge 1/4$, then $\mathbb{P}(Z \ge 1/8) \ge 1/7$. Indeed, $1/4 \le \mathbb{E}[Z] \le \mathbb{P}(Z < 1/8)/8 + \mathbb{P}(Z \ge 1/8) = 1/8 - 7 \mathbb{P}(Z \ge 1/8)/8$. All the X-samples S_1^{X}, \ldots, S_k^{X} , for $k = (2n)^n$, are equaly likely. For $1 \le j \le k$, if $S_j^{X} = (x_1, \ldots, x_n)$ we denote by $S_j^{I} = ((x_1, f_i(x_1)), \ldots, (x_n, f_i(x_n)), \operatorname{and} \tilde{f}_j = A(S_j^{I})$. $\max_{1 \le i \le T} \mathbb{E}[\iota_{D_i}(A(S))] = \max_{1 \le i \le T} \frac{1}{k} \sum_{j=1}^k \iota_{D_i}(\tilde{f}_j^{I}) \ge \frac{1}{\tau} \sum_{i=1}^T \frac{1}{k} \sum_{j=1}^k \iota_{D_i}(\tilde{f}_j^{I}) = \frac{1}{k} \sum_{j=1}^K \frac{1}{\tau} \sum_{i=1}^T \iota_{D_i}(\tilde{f}_j^{I}) \ge \min_{1 \le i \le T} \frac{1}{\tau} \iota_{D_i}(\tilde{f}_j^{I})$.

$$\begin{aligned} \text{Fix } 1 &\leq j \leq \textit{k, denote } S_j^{X} = (x_1, \dots, x_n) \text{ and define } \{v_1, \dots, v_p\} = \mathcal{C} \setminus \{x_1, \dots, x_n\}, \text{ where } p \geq \textit{n. Then} \\ & \mathcal{L}_{D_i} \binom{j_i}{j} = \frac{1}{2n} \sum_{x \in \mathcal{C}} \mathbbm{1} \{l_j^j(x) \neq f_i(x)\} \geq \frac{1}{2p} \sum_{r=1}^p \mathbbm{1} \{l_j^j(v_r) \neq f_i(v_r)\} \\ \text{and hence} & \frac{1}{\tau} \sum_{i=1}^T \mathcal{L}_{D_i} \binom{j_i}{l_j} \geq \frac{1}{\tau} \sum_{r=1}^T \frac{1}{2p} \sum_{r=1}^p \mathbbm{1} \{l_j^j(v_r) \neq f_i(v_r)\} \geq \frac{1}{2} \min_{1 \leq i \leq p} \frac{1}{\tau} \sum_{i=1}^T \mathbbm{1} \{l_j^j(v_r) \neq f_i(v_r)\} \\ \end{aligned}$$

Fix $1 \leq r \leq p$. Then the functions $\{f_i : 1 \leq i \leq T\}$ can be grouped into T/2 pairs of functions $(\int_{t_i}^{D}, \int_{t_i}^{T_i}), 1 \leq i \leq T/2$ which agree on all $x \in C$ except on v_r , and for all $1 \leq i \leq T/2$ it holds that $\{J_{f_i}^{j}(v_r) \neq \tilde{I}_{i}^{0}(v_r)\} + 1\{J_{f_i}^{j}(v_r) \neq \tilde{I}_{i}^{1}(v_r)\} = 1$. Hence,

$$\sum_{j=1}^{T} \mathbb{1}\left\{ \vec{j}_{j}(\mathbf{v}_{r}) \neq f_{i}(\mathbf{v}_{r}) \right\} = \sum_{i=1}^{T/2} \mathbb{1}\left\{ \vec{j}_{j}(\mathbf{v}_{r}) \neq \vec{j}_{i}^{0}(\mathbf{v}_{r}) \right\} + \mathbb{1}\left\{ \vec{j}_{j}(\mathbf{v}_{r}) \neq \vec{j}_{i}^{1}(\mathbf{v}_{r}) \right\} = T/2, \text{ which concludes the proof.}$$





Consequence: infinite VC-dimension \implies no learnability

Recall that a hypothesis class \mathcal{H} is *agnostic PAC learnable* if there exists a function $n_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ and a learning algorithm $S \mapsto \hat{h}_n$ such that for every $\epsilon, \delta \in (0,1)$, for every distribution D on $\mathcal{X} \times \mathcal{Y}$ when $S = ((X_1, Y_1), \dots, (X_n, Y_n)) \stackrel{iid}{\sim} D$,

$$\mathbb{P}\Big(L_{D}(\hat{h}_{n}) \geq \min_{h' \in \mathcal{H}} L_{D}(h') + \epsilon\Big) \leq \delta$$

for all $n \ge n_{\mathcal{H}}(\epsilon, \delta)$.

Theorem

Let ${\mathcal H}$ be a class of infinite VC-dimension. Then ${\mathcal H}$ is not PAC-learnable.

Proof: for every training size *n*, there exists a set $C \subset \mathcal{X}$ of size 2n that is shattered by \mathcal{H} . By the NFL theorem, for every learning algorithm *A* there exists a probability distribution *D* over $\mathcal{X} \times \{0, 1\}$ and $h : \mathcal{X} \to \{0, 1\}$ such that $L_D(h) = 0$ but with probability at least 1/7 over the training set, we have $L_D(A(S)) \ge 1/8$.





Consequence: Curse of Dimensionality

Theorem

Let c > 1 be a Lipschitz constant. Let A be any learning algorithm for binary classification over a domain $\mathcal{X} = [0, 1]^d$. If the training set size is $n \leq (c + 1)^d/2$, then there exists a distribution \mathcal{D} over $[0, 1]^d \times \{0, 1\}$ such that:

- $\eta(\mathbf{x}) = \mathbb{P}(\mathbf{Y} = 1 | \mathbf{X} = \mathbf{x})$ is c-Lipschitz;
- the Bayes error of the distribution is 0;
- with probability at least 1/7 over the choice of S $\sim \mathcal{D}^{\otimes n}$,

 $L_{\mathcal{D}}(A(S)) \geq \frac{1}{8}$.



Shattering

Definition

Let \mathcal{H} be a class of functions $\mathcal{X} \to \{0, 1\}$ and let $C = \{x_1, \dots, x_m\} \subset \mathcal{X}$. The *restriction* of \mathcal{H} to C is the set of functions $C \to \{0, 1\}$ that can be derived from \mathcal{H} :

$$\mathcal{H}_{C} = \left\{ (x_{1}, \ldots, x_{m}) \rightarrow (h(x_{1}), \ldots, h(x_{m})) : h \in \mathcal{H} \right\}.$$

Shattering

h

A hypothesis class \mathcal{H} shatters a finite set $C \subset \mathcal{X}$ if $\mathcal{H}_{C} = \{0, 1\}^{C}$. Example:

•
$$\mathcal{H} = \{\mathbb{1}_{]-\infty,a]} : a \in \mathbb{R}\}.$$

• $\mathcal{H}_{rec}^2 = \{h_{(a_1,b_1,a_2,b_2)} : a_1 \le b_1 \text{ and } a_2 \le b_2\}$ where

$$(a_1,b_1,a_2,b_2)(x_1,x_2) = \begin{cases} 1 & \text{if } a_1 \leq x_1 \leq b_1 \text{ and } a_2 \leq x_2 \leq b_2; \\ 0 & \text{otherwise }. \end{cases}$$





VC dimension

Definition

The Vapnik Chervonenkis dimension $\operatorname{VCdim}(\mathcal{H})$ of a hypothesis class \mathcal{H} is the maximal size of a set $\mathcal{C} \subset \mathcal{X}$ that can be shattered by \mathcal{H} . If \mathcal{H} can shatter sets of arbitrarily large size we say that $\operatorname{VCdim}(\mathcal{H}) = \infty$.

Example:

•
$$\mathcal{H} = \{\mathbb{1}_{]-\infty,a]} : a \in \mathbb{R}\}.$$

•
$$\mathcal{H}^2_{\text{rec}} = \left\{ \mathbb{R}^2 \ni \mathsf{x} \mapsto \mathbb{1}_{[a_1, b_1]}(\mathsf{x}_1) \mathbb{1}_{[a_2, b_2]}(\mathsf{x}_2) : a_1 \le b_1 \text{ and } a_2 \le b_2 \right\}$$



Fundamental theorem of PAC learning

Let \mathcal{H} be a hypothesis class of functions from a domain \mathcal{X} to $\{0,1\}$ and let the loss function of 0-1 loss. Then the following propositions are equivalent:

- 1. ${\mathcal H}$ has the uniform convergence property,
- 2. any ERM rule is a successful agnostic PAC learner for $\mathcal{H},$
- 3. $\mathcal H$ is agnostic PAC learnable,
- 4. \mathcal{H} has finite VC-dimension.



Fundamental theorem of PAC learning (quantitative version)

Let \mathcal{H} be a hypothesis class of functions from a domain \mathcal{X} to $\{0, 1\}$ and let the loss function of 0 - 1 loss. Assume that $d := \text{VCdim}(\mathcal{H}) < \infty$. Then there exist constants C_1, C_2 such that:

1. ${\mathcal H}$ has the uniform convergence property with sample complexity

$$\mathsf{C}_1 \frac{\mathsf{d} + \log(1/\delta)}{\epsilon^2} \le \mathsf{n}_{\mathcal{H}}^{\mathsf{UC}}(\epsilon, \delta) \le \mathsf{C}_2 \frac{\mathsf{d} + \log(1/\delta)}{\epsilon^2} \;,$$

2. ${\mathcal H}$ is agnostic PAC learnable with sample complexity

$$\mathsf{C}_1 rac{d + \log(1/\delta)}{\epsilon^2} \leq \mathsf{n}_{\mathcal{H}}(\epsilon, \delta) \leq \mathsf{C}_2 rac{d + \log(1/\delta)}{\epsilon^2} \; ,$$



Sauer's lemma

Definition

Let \mathcal{H} be a hypothesis class. Then the *growth function* of \mathcal{H} , denoted $\tau_{\mathcal{H}} : \mathbb{N} \to \mathbb{N}$, is defined as the maximal number of different functions that can be obtained by restricting \mathcal{H} to a set of size m: $\tau_{\mathcal{H}}(m) = \max_{C \subset \mathcal{X}: |C| = m} |\mathcal{H}_{C}|$.

Note: if $\operatorname{VCdim}(\mathcal{H}) = d$, then for any $m \leq d$ we have $\tau_{\mathcal{H}}(m) = 2^m$.

Sauer's lemma

Let $\mathcal H$ be a hypothesis class with $d = \mathrm{VCdim}(\mathcal H) < \infty$. Then, for all $m \geq d$,

$$au_{\mathcal{H}}(m) \leq \sum_{i=0}^d \binom{m}{i} \leq \left(\frac{em}{d}\right)^d \; .$$

Think of example: $\mathcal{H} = \left\{ \mathbb{1}_{(-\infty,a]} : a \in \mathbb{R} \right\}$ with $d = \operatorname{VCdim}(\mathcal{H}) = 1$.



Proof of Sauer's lemma 1/2

In fact we prove the stronger claim:

$$|\mathcal{H}_{C}| \leq |\{B \subset C : \mathcal{H} \text{ shatters } B\}| \leq \sum_{i=0}^{d} {m \choose i}.$$

where the last inequality holds since no set of size larger than d is shattered by \mathcal{H} . The proof is by induction.

m=1: The empty set is always considered to be shattered by \mathcal{H} . Hence, either $|\mathcal{H}_{\mathcal{L}}| = 1$ and d = 0, inequality $1 \leq 1$, or $d \geq 1$ and the inequality is $2 \leq 2$. **Induction:** Let $C = \{x_1, \ldots, x_m\}$, and let $C' = \{x_2, \ldots, x_m\}$. We note functions like vectors, and we define

$$\begin{split} & r_0 \, = \, \Big\{ (y_2 \,, \, \ldots \,, y_m) \, : \, (0, y_2 \,, \, \ldots \,, y_m) \, \in \, \mathcal{H}_{\mathcal{C}} \, \text{or} \, (1, y_2 \,, \, \ldots \,, y_m) \, \in \, \mathcal{H}_{\mathcal{C}} \Big\}, \quad \text{and} \\ & r_1 \, = \, \Big\{ (y_2 \,, \, \ldots \,, y_m) \, : \, (0, y_2 \,, \, \ldots \,, y_m) \, \in \, \mathcal{H}_{\mathcal{C}} \, \text{and} \, (1, y_2 \,, \, \ldots \,, y_m) \, \in \, \mathcal{H}_{\mathcal{C}} \Big\} \,. \end{split}$$

Then $|\mathcal{H}_{C}| = |Y_{0}| + |Y_{1}|$. Moreover, $Y_{0} = \mathcal{H}_{C'}$ and hence by the induction hypothesis:

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$$|Y_0| = |\mathcal{H}_{\mathcal{C}'}| \le |\{B' \subset \mathcal{C}' : \mathcal{H} \text{ shatters } B'\}| = |\{B \subset \mathcal{C} : x_1 \notin B \text{ and } \mathcal{H} \text{ shatters } B\}|$$

Next, define

$$\mathcal{H}' = \left\{ h \in \mathcal{H} : \exists h' \in \mathcal{H} \text{ s.t. } \forall 1 \leq i \leq m, h'(x_i) = \left| \begin{array}{c} 1 - h(x_1) \text{ if } i = 1 \\ h(x_i) \text{ otherwise} \end{array} \right\} \right\}$$

Note that \mathcal{H}' shatters $B' \subset C'$ iff \mathcal{H}' shatters $B' \cup \{x_1\}$, and that $Y_1 = \mathcal{H}'_{C'}$. Hence, by the induction hypothesis,

$$\begin{split} |Y_1| &= |\mathcal{H}'_{\mathcal{C}'}| \leq |\{B' \subset \mathcal{C}' : \mathcal{H}' \text{ shatters } B'\}| = |\{B' \subset \mathcal{C}' : \mathcal{H}' \text{ shatters } B' \cup \{x_1\}\}| \\ &= |\{B \subset \mathcal{C} : x_1 \in B \text{ and } \mathcal{H}' \text{ shatters } B\}| \leq |\{B \subset \mathcal{C} : x_1 \in B \text{ and } \mathcal{H} \text{ shatters } B\}| \;. \end{split}$$

Overall,

$$\left|\mathcal{H}_{C}\right| = \left|Y_{0}\right| + \left|Y_{1}\right| \leq \left|\left\{B \subset C : x_{1} \notin B \text{ and } \mathcal{H} \text{ shatters } B\right\}\right| + \left|\left\{B \subset C : x_{1} \in B \text{ and } \mathcal{H} \text{ shatters } B\right\}\right| = \left|\left\{B \subset C : \mathcal{H} \text{ shatters } B\right\}\right|.$$



Proof of Sauer's lemma 2/2

For the last inequality, one may observe that if $m \ge 2d$, defining $N \sim B(m, 1/2)$, Chernoff's inequality and inequality $\log(u) \ge (u-1)/u$ yield

$$-\log \mathbb{P}(N \le d) \ge m \operatorname{kl}\left(\frac{d}{m}, \frac{1}{2}\right) \ge d \log \frac{2d}{m} + (m-d) \log \frac{2(m-d)}{m}$$
$$\ge m \log(2) + d \log \frac{d}{m} + (m-d) \frac{-d/m}{(m-d)/m} = m \log(2) + d \log \frac{d}{em}$$

and hence

$$\sum_{i=0}^{d} \binom{m}{i} = 2^{m} \mathbb{P}(N \le d) \le \exp\left(-d\log\frac{d}{em}\right) = \left(\frac{em}{d}\right)^{d}$$

Besides, for the case $d \le m \le 2d$, the inequality is obvious since $(em/d)^d \ge 2^m$: indeed, function $f : x \mapsto -x \log(x/e)$ is increasing on [0, 1], and hence for all $d \le m \le 2d$:

$$\frac{d}{m}\log\frac{em}{d} = f(d/m) \ge f(1/2) = \frac{1}{2}\log(2e) \ge \log(2) ,$$

which implies $\left(\frac{em}{d}\right)^d = \exp\left(d\log\frac{em}{d}\right) \geq \exp(m\log(2)) = 2^m$. Alternately, you may simply observe that for all $m \geq d$,

$$\left(\frac{d}{m}\right)^d \sum_{i=0}^d \binom{m}{i} \le \sum_{i=0}^d \left(\frac{d}{m}\right)^i \binom{m}{i} \le \sum_{i=0}^m \left(\frac{d}{m}\right)^i \binom{m}{i} = \left(1 + \frac{d}{m}\right)^m \le e^d \; .$$





Finite VC dimension implies Uniform Convergence

Theorem

Let \mathcal{H} be a class and let $\tau_{\mathcal{H}}$ be its growth function. Then, for every distribution D dans for every $\delta \in (0, 1)$, with probability at least $1 - \delta$ over the choice of the sample $S \sim D^{\otimes n}$ we have

$$\sup_{h \in \mathcal{H}} \left| \mathcal{L}_{\mathcal{D}}(h) - \mathcal{L}_{\mathcal{S}}(h) \right| \leq \frac{1 + \sqrt{\log\left(\tau_{\mathcal{H}}(2n)\right)}}{\delta \sqrt{n/2}}$$

Note: this result is sufficient to prove that finite VC-dim \implies learnable, but the dependency in δ is not correct at all: roughly speaking, the factor $1/\delta$ can be replaced by $\log(1/\delta)$.



Proof: symmetrization and Rademacher complexity (1/2)

We consider the 0-1 loss $\ell(h, (x, y)) = \mathbb{1}\{h(x) \neq y\}$, or any [0, 1]-valued loss ℓ . We denote $Z_i = (X_i, Y_i)$, and observe that $L_D(h) = \mathbb{E}_{Z_i}[\ell(h, Z_i)] = \mathbb{E}_{S'}[L_{S'}(h)]$ if $S' = Z'_1, \ldots, Z'_n$ denotes another iid sample of D. Hence,

$$\begin{split} \mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| L_{D}(h) - L_{S}(h) \right| \right] &= \mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{S'} \left[L_{S'}(h) \right] - L_{S}(h) \right| \right] = \mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{S'} \left[L_{S'}(h) - L_{S}(h) \right] \right| \right] \\ &\leq \mathbb{E}_{S} \left[\sup_{h \in \mathcal{H}} \mathbb{E}_{S'} \left[\left| L_{S'}(h) - L_{S}(h) \right| \right] \right] \leq \mathbb{E}_{S} \left[\mathbb{E}_{S'} \left[\sup_{h \in \mathcal{H}} \left| L_{S'}(h) - L_{S}(h) \right| \right] \right] \\ &= \mathbb{E}_{S,S'} \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \left| \sum_{i=1}^{n} \ell(h, Z'_{i}) - \ell(h, Z_{i}) \right| \right] \\ &= \mathbb{E}_{S,S'} \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \left| \sum_{i=1}^{n} \sigma_{i} (\ell(h, Z'_{i}) - \ell(h, Z_{i})) \right| \right] \quad \text{for all } \sigma \in \{\pm 1\}^{n} \\ &= \mathbb{E}_{\Sigma} \mathbb{E}_{S,S'} \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \left| \sum_{i=1}^{n} \Sigma_{i} (\ell(h, Z'_{i}) - \ell(h, Z_{i})) \right| \right] \quad \text{if } \Sigma \sim \mathcal{U}(\{\pm 1\}^{n}) \\ &= \mathbb{E}_{S,S'} \mathbb{E}_{\Sigma} \left[\sup_{h \in \mathcal{H}} \frac{1}{n} \left| \sum_{i=1}^{n} \Sigma_{i} (\ell(h, Z'_{i}) - \ell(h, Z_{i})) \right| \right] \quad . \end{split}$$





Proof: symmetrization and Rademacher complexity (1/2)

We consider the 0-1 loss $\ell(h, (x, y)) = \mathbb{1}\{h(x) \neq y\}$, or any [0, 1]-valued loss ℓ . We denote $Z_i = (X_i, Y_i)$, and observe that $L_D(h) = \mathbb{E}_{Z_i}[\ell(h, Z_i)] = \mathbb{E}_{S'}[L_{S'}(h)]$ if $S' = Z'_1, \ldots, Z'_n$ denotes another iid sample of D. Hence,

$$\begin{split} \mathbb{E}_{\mathsf{S}}\left[\sup_{h\in\mathcal{H}}\left|L_{\mathsf{D}}(h)-L_{\mathsf{S}}(h)\right|\right] &= \mathbb{E}_{\mathsf{S}}\left[\sup_{h\in\mathcal{H}}\left|\mathbb{E}_{\mathsf{S}'}[L_{\mathsf{S}'}(h)]-L_{\mathsf{S}}(h)\right|\right] = \mathbb{E}_{\mathsf{S}}\left[\sup_{h\in\mathcal{H}}\left|\mathbb{E}_{\mathsf{S}'}\left[L_{\mathsf{S}'}(h)-L_{\mathsf{S}}(h)\right]\right|\right] \\ &= \mathbb{E}_{\mathsf{S},\mathsf{S}'}\mathbb{E}_{\Sigma}\left[\sup_{h\in\mathcal{H}}\frac{1}{n}\left|\sum_{i=1}^{n}\Sigma_{i}\left(\ell(h,Z'_{i})-\ell(h,Z_{i})\right)\right|\right] \,. \end{split}$$

Now, for every S, S', let $C = C_{S,S'} = \{x : \exists i \in \{1, \dots, n\} : x = X_i \text{ or } X'_i\}$. Then $\forall \sigma \in \{-1, 1\}^n$,

$$\sup_{h \in \mathcal{H}} \frac{1}{n} \left| \sum_{i=1}^{n} \sigma_i \left(\ell(h, Z'_i) - \ell(h, Z_i) \right) \right| = \max_{h \in \mathcal{H}_c} \frac{1}{n} \left| \sum_{i=1}^{n} \sigma_i \left(\ell(h, Z'_i) - \ell(h, Z_i) \right) \right| .$$



Proof: symmetrization and Rademacher complexity (2/2)

Moreover, for every $h \in \mathcal{H}_{\mathcal{C}}$ let $Z_h = \frac{1}{n} \sum_{i=1}^n \Sigma_i (\ell(h, Z'_i) - \ell(h, Z_i))$. Then $\mathbb{E}_{\Sigma}[Z_h] = 0$, each summand belongs to [-1, 1] and by Hoeffding's inequality, for every $\epsilon > 0$:

$$\mathbb{P}_{\Sigma}\left[|Z_{h}| \geq \epsilon\right] \leq 2 \exp\left(-\frac{n\epsilon^{2}}{2}\right)$$

Hence, by the union bound,

$$\mathbb{P}_{\Sigma}ig[\max_{h\in\mathcal{H}_{\mathcal{C}}}|Z_{h}|\geq\epsilonig]\leq 2ig|\mathcal{H}_{\mathcal{C}}ig|\exp\left(-rac{n\epsilon^{2}}{2}
ight)\;.$$

The following lemma permits to deduce that

$$\mathbb{E}_{\Sigma}\left[\max_{h \in \mathcal{H}_{\mathcal{L}}} |Z_{h}|\right] \leq \frac{1 + \sqrt{\log(|\mathcal{H}_{\mathcal{L}}|)}}{\sqrt{n/2}} \leq \frac{1 + \sqrt{\log(\tau_{\mathcal{H}}(2n))}}{\sqrt{n/2}}$$

since $|C| \leq 2n$. Hence,

$$\mathbb{E}_{S}\left[\sup_{h\in\mathcal{H}}\left|\mathcal{L}_{D}(h)-\mathcal{L}_{S}(h)\right|\right] \leq \mathbb{E}_{S,S'}\mathbb{E}_{\Sigma}\left[\sup_{h\in\mathcal{H}}\frac{1}{n}\left|\sum_{i=1}^{n}\Sigma_{i}\left(\ell(h,Z_{i}')-\ell(h,Z_{i})\right)\right|\right] \leq \frac{1+\sqrt{\log(\tau_{\mathcal{H}}(2n))}}{\sqrt{n/2}},$$

and we conclude by using Markov's inequality (poor idea! Better: McDiarmid's inequality).



Technical Lemma

Lemma

Let a > 0, b > 1, and let Z be a real-valued random variable such that for all t > 0, $\mathbb{P}(Z \ge t) \le 2b \exp\left(-\frac{t^2}{a^2}\right). \text{ Then}$ $\mathbb{E}[Z] \le a\left(\sqrt{\log(b)} + \frac{1}{\sqrt{\log(b)}}\right).$ $\mathbb{E}[Z] \le \int_{0}^{\infty} \mathbb{P}(Z \ge t) dt \le a \sqrt{\log(b)} + \int_{1}^{\infty} 2b \exp\left(-\frac{t^{2}}{a^{2}}\right) dt$ Proof: $\leq a\sqrt{\log(b)} + 2b\int_{q_{\star}/\log(b)}^{\infty} \frac{t}{q_{\star}/\log(b)} \exp\left(-\frac{t^2}{a^2}\right) dt$ $=a\sqrt{\log(b)} + \frac{2b}{a\sqrt{\log(b)}} \times \frac{a^2}{2} \exp\left(-\frac{(a\sqrt{\log(b)})^2}{a^2}\right)$ $=a\sqrt{\log(b)}+\frac{a}{\sqrt{\log(b)}}$.

NB: cutting at $a\sqrt{\log(2b)}$ gives a better but less nice inequality for our use.



Application: Finite VC-dim classes are agnostically learnable

It suffices to prove that finite VC-dim implies the uniform convergence property. From Sauer's lemma, for all $m \ge d/2$ we have $\tau_{\mathcal{H}}(2n) \le (2en/d)^d$. With the previous theorem, this yields that with probability at least $1 - \delta$:

$$\sup_{h \in \mathcal{H}} \left| \mathcal{L}_{D}(h) - \mathcal{L}_{S}(h) \right| \leq \frac{1 + \sqrt{d \log \left(2en/d \right)}}{\delta \sqrt{n/2}} \leq \frac{1}{\delta} \sqrt{\frac{8d \log(2en/d)}{n}}$$

as soon as $\sqrt{d\log\left(2en/d
ight)} \geq 1.$ To ensure that this is at most ϵ , one may choose

$$n \ge \frac{8d\log(n)}{(\delta\epsilon)^2} + \frac{8d\log(2e/d)}{(\delta\epsilon)^2}$$

By the following lemma, it is sufficient that



Technical Lemma

Lemma

Let a > 0. Then

$$x \ge 2a\log(a) \implies x \ge a\log(x)$$
.

Proof: For $a \le e$, true for every x > 0. Otherwise, for $a \ge \sqrt{e}$ we have $2a\log(a) \ge a$ and thus for every $t \ge 2a\log(a)$, as $f : t \mapsto t - a\log(t)$ is increasing on $[a, \infty)$, $f(t) \ge f(2a\log(a)) = a\log(a) - a\log(2\log(a)) \ge 0$, since for every a > 0 it holds that $a \ge 2\log(a)$.

Lemma Let $a \ge 1, b > 0$. Then

$$x \ge 4a \log(2a) + 2b \implies x \ge a \log(x) + b$$
.

Proof: It suffices to check that $x \ge 2a \log(x)$ (given by the above lemma) and that $x \ge 2b$ (obvious since $4a \log(2a) \ge 0$).

