Statistical Machine Learning

https://cvml.ist.ac.at/courses/SML_W18

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Lecture 8

Overview (tentative)

Date		no.	Topic
Oct 08	Mon	1	A Hands-On Introduction
Oct 10	Wed	–	self-study (Christoph traveling)
Oct 15	Mon	2	Bayesian Decision Theory
			Generative Probabilistic Models
Oct 17	Wed	3	Discriminative Probabilistic Models
			Maximum Margin Classifiers
Oct 22	Mon	4	Generalized Linear Classifiers, Optimization
Oct 24	Wed	5	Evaluating Predictors; Model Selection
Oct 29	Mon	–	self-study (Christoph traveling)
Oct 31	Wed	6	Overfitting/Underfitting, Regularization
Nov 05	Mon	7	Learning Theory I: classical/Rademacher bounds
Nov 07	Wed	8	Learning Theory II: miscellaneous
Nov 12	Mon	9	Probabilistic Graphical Models I
Nov 14	Wed	10	Probabilistic Graphical Models II
Nov 19	Mon	11	Probabilistic Graphical Models III
Nov 21	Wed	12	Probabilistic Graphical Models IV
until Nov 25			final project

Beyond complexity measures

Algorithm-dependent bounds

Generalization bounds so far: with probability at least $1 - \delta$:

$$\forall f \in \mathcal{H}: \quad \mathcal{R}(f) \leq \hat{\mathcal{R}}(f) + \text{"something"}$$

Observation:

- holds simultaneous for all hypotheses in $\mathcal{H}$, we can pick any we like

  but: in practice, we have some algorithm that choses the hypothesis and really only need the result for that

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Goal: algorithm-dependent bounds

Instead of

- *"For which hypothesis sets does learning not overfit?"*

ask

- *"Which learning algorithms do not overfit?"*

- $\mathcal{Z}$: input set (typically $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$)
- $\mathcal{H}$: set of hypotheses
- $L(h, z)$: loss function of the form $L(h, z) = \ell(y, f(x))$

Definition (Learning algorithm)

A **learning algorithm**, A, is a function that takes as input a finite subset, $\mathcal{D}_m \subset \mathcal{Z}$, and outputs a hypothesis $A[\mathcal{D}] \in \mathcal{H}$.

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Definition (Uniform stability)

For a training set, $\mathcal{D} = \{z_1, \ldots, z_m\}$, we call the training set with the i-th element removed $\mathcal{D}^{\setminus i} = \{z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_m\}$.

A learning algorithm, A, has **uniform stability** β with respect to the loss ℓ if the following holds,

$$\forall \mathcal{D}_m \subset \mathcal{Z}\ \forall i \in \{1, 2, \ldots, m\} \qquad \|L(A[\mathcal{D}], \cdot) - L(A[\mathcal{D}^{\setminus i}], \cdot)\|_\infty \leq \beta$$

For a uniformly stable algorithm, changing the training set a little has only a small effect.

Theorem (Stable algorithms generalize well [Bousquet *et al.*, 2002])

Let A be a β-uniformly stable learning algorithm. For a training set $\mathcal{D}$ that consists of m i.i.d. samples, denote by $f = A[\mathcal{D}]$ be the output of A on $\mathcal{D}$. Let $\ell(y, \bar{y})$ be bounded by M.

Then, for any $\delta > 0$, with probability at least $1 - \delta$,

$$\mathcal{R}(f) \leq \hat{\mathcal{R}}(f) + 2\beta + (4m\beta + M)\sqrt{\frac{\log(1/\delta)}{2m}}$$

Bound is useful, if stability β behaves (at least) like $\frac{1}{m}$.

Stochastic gradient descent (SGD): minimize a function

$$f(\theta) = \frac{1}{m} \sum_{i=1}^{m} f(\theta; z_i)$$

Theorem (Stability of Stochastic Gradient Descent [Hardt *et al.*, 2016])

Let $f(\cdot, z)$ be γ-smooth, convex and L-Lipschitz for every z. Suppose that we run SGD with step sizes $\alpha_t \leq 2/\gamma$ for T steps. Then, SGD satisfies uniform stability with

$$\beta \leq \frac{2L^2}{m} \sum_{t=1}^{T} \alpha_t.$$

Let $f(\cdot, z)$ be γ-smooth and L-Lipschitz, but not necessarily convex. Assume we run SGD with monotonically non-increasing step sizes $\alpha_t \leq c/t$ for some c. Then, SGD satisfies uniform stability with

$$\beta \leq \frac{1 + \frac{1}{\gamma c}}{m - 1} (2cL^2)^{\frac{1}{\gamma c + 1}} T^{\frac{\gamma c}{\gamma c + 1}}.$$

The power of compression

Reminder:

Perceptron – Training

input training set $\mathcal{D} \subset \mathbb{R}^d \times \{-1, +1\}$
  initialize $w = (0, \ldots, 0) \in \mathbb{R}^d$.
  repeat
    for all $(x, y) \in \mathcal{D}$: **do**
      compute $a := \langle w, x \rangle$ ('activation')
      if $ya \leq 0$ **then**
        $w \leftarrow w + yx$
      end if
    end for
  until w wasn't updated for a complete pass over $\mathcal{D}$

Let's assume $\mathcal{D}$ is very large, so we don't need multiple passes.
Properties:

- sequential training, one pass over data
- only those examples matter, where perceptron made a mistake (only those lead to changes of w)

Towards Sample Compression Bounds

- Take training set as a sequence:

$$T = ((x^1, y^1), (x^2, y^2), \ldots, (x^n, y^n))$$

- algorithm A processes T in order, producting output $f := A(T)$
- What only a subset of examples influence the algorithm output?
- for increasing subsequence, $I \subset \{1, \ldots, n\}$, with $|I| = l$, set

$$T_I = ((x^{i_1}, y^{i_1}), (x^{i_2}, y^{i_2}), \ldots, (x^{i_l}, y^{i_l}))$$

Definition

I is a **compression set** for T, if $A(T) = A(T_I)$.

Example: $I = \{$set of examples where Perceptron made a mistake$\}$

Definition (Compression scheme [Littlestone/Warmuth, 1986])

A learning algorithm A is called **compression scheme**, if there is a pair of functions: C (called compression function), and L (called reconstruction function), such that:

- C takes as input a finite dataset and outputs a subsequence of indices
- L takes as input a finite dataset and outputs a predictor
- A is the result of applying L to the data selected by C

$$A = L(T_I) \text{ for } I = C(T)$$

Examples:

- Perceptron ($I =$ indices of examples where will be updated)
- SVMs ($I =$ set of support vectors)
- k-NN ($I =$ set of examples that support the decision boundaries)

$$\hat{\mathcal{R}}_I(h) = \frac{1}{|I|}\sum_{i\in I}\ell(\,y^i, h(x^i)\,) \quad \text{and} \quad \hat{\mathcal{R}}_{\neg I}(h) = \frac{1}{n-|I|}\sum_{i\notin I}\ell(\,y^i, h(x^i)\,)$$

Theorem (Compression Bound [Littlestone/Warmuth, 1986; Graepel 2005])

Let A be a compression scheme with compression function C. Let the loss ℓ be bounded by $[0,1]$. Then, with probability at least $1-\delta$ over the random draw of T, we have that:

If $\hat{\mathcal{R}}_{\neg I}(A(T)) = 0$:

$$\mathcal{R}(A(T)) \leq \frac{1}{m-l}\big(\,(l+1)\log m + \log\frac{1}{\delta}\big).$$

For general $\hat{\mathcal{R}}_{\neg I}(A(T))$:

$$\mathcal{R}(A(T)) \leq \frac{m}{m-l}\hat{\mathcal{R}}_{\neg I}(A(T)) + \sqrt{\frac{(l+2)\log m + \log\frac{1}{\delta}}{2(m-l)}}$$

where $I = C(T)$ and $l = |I|$.

The power of randomization

The problem of overfitting emerges mainly because we pick only a single classifier, h, and just by accident it can have $\mathcal{R}(h) \gg \hat{\mathcal{R}}(h)$.
If we choose many classifiers and combine their decisions, chances of overfitting should be lower.

Definition (Majority-vote)

Let $\mathcal{Y} = \{\pm 1\}$ (only for convenience of notation). Let $h_1, \ldots, h_T \in \mathcal{H}$ be a set of hypotheses. We define the **uniform majority vote** classifier as

$$h_{\text{majority}}(x) = \operatorname{sign} \frac{1}{T} \sum_{i=1}^{T} h_i(x)$$

Definition (Majority-vote)

More generally, for weights $\alpha_i \in [0,1]$, $\sum_i \alpha_i = 1$, the α-**weighted majority vote classifier** is:

$$h^{\alpha}_{\text{majority}}(x) = \operatorname{sign} \sum_{i=1}^{T} \alpha_i h_i(x) = \mathop{\mathbb{E}}_{i \sim \alpha} [h_i(x)]$$

Weighting make a convenient framework:

- we can use a base set of many (even countably infinite) classifier
- we assign weights to *good classifiers*, e.g. based on training data
- classical setting is included: for $\alpha = \delta_{i=j}$: $\quad h^{\alpha}_{\text{majority}} = h_j$

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Unfortunately, majority vote classifiers are not easy to classify:

- classical bounds hold equally for *any* $h \in \mathcal{H}$
- if $h^{\alpha}_{\text{majority}} \in \mathcal{H}$, bound no better than for others
- if $h^{\alpha}_{\text{majority}} \notin \mathcal{H}$, no bound at all

Trick: analyze stochastic classifiers

Stochastic Classifiers

Standard scenario:

- $\mathcal{X}$: input set, $\mathcal{Y}$: output set, p probability distribution over $\mathcal{X} \times \mathcal{Y}$
- $\mathcal{H} \subset \{\mathcal{X} \to \mathcal{Y}\}$: hypothesis set, ℓ: loss function
- $\mathcal{D} = \{(x^1, y^1) \ldots, (x^n, y^n)\} \overset{i.i.d.}{\sim} p(x, y)$: training set

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New:

- Q probability distribution over $\mathcal{H}$

Definition (Gibbs classifier)

For a distribution Q over $\mathcal{H} \subset \{h : \mathcal{X} \to \mathcal{Y}\}$, the **Gibss classifier**, h_Q, is defined by the procedure:

- input: $x \in \mathcal{X}$
- sample $h \sim Q$
- output: $h(x)$

The Gibbs classifier is a stochastic classifier, its output is a random variable (wrt Q).

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Because the classifier output is random, so are the risks:

$$\mathcal{R}(h_Q) = \mathop{\mathbb{E}}_{(x,y)\sim p} \ell(y, h_Q(x)) \qquad \hat{\mathcal{R}}(h_Q) = \sum_{i=1}^{n} \ell(y^i, h_Q(x^i))$$

We can study their expected value:

$$\mathcal{R}(Q) = \mathop{\mathbb{E}}_{h\sim Q} \mathcal{R}(h) = \mathop{\mathbb{E}}_{h\sim Q} \mathop{\mathbb{E}}_{(x,y)\sim p} \ell(y, h(x)) \qquad \hat{\mathcal{R}}(Q) = \mathop{\mathbb{E}}_{h\sim Q} \sum_{i=1}^{n} \ell(y^i, h(x^i))$$

Learning

- $\mathcal{X}$: input set, $\mathcal{Y}$: output set, p probability distribution over $\mathcal{X} \times \mathcal{Y}$
- $\mathcal{H} \subset \{\mathcal{X} \to \mathcal{Y}\}$: hypothesis set, ℓ: loss function

What's the analog of deterministic learning?

Given a training set, $\mathcal{D} = \{(x^1, y^1) \ldots, (x^n, y^n)\} \overset{i.i.d.}{\sim} p(x, y)$, identify a distribution Q (arbitrary, or from a parametric family), such that $\mathcal{R}(Q)$ is as small as possible.

What would a generalization bound look like?

$$\mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \text{"something"}$$

Gibbs classifier vs. majority vote

Majority vote classifier: (now calling weights Q instead of α)

- evaluate all classifiers, $h(x)$ for $h \in \mathcal{H}$
- combine their outputs according to their weights, $\mathbb{E}_{h\sim Q}\, h(x)$
- make one decision based on the result, $\operatorname{sign} \mathbb{E}_{h\sim Q}\, h(x)$
- evaluate the loss of this decision, $\ell(y, \operatorname{sign} \mathbb{E}_{h\sim Q}\, h(x))$

Gibbs classifier:

- evaluate all classifiers, $h(x)$ for $h \in \mathcal{H}$
- evaluate the loss of all their decisions, $\ell(y, h(x))$ for $h \in \mathcal{H}$
- combine their losses according to their weights, $\mathbb{E}_{h\sim Q}\, \ell(y, h(x))$

How are the two situations related?

Lemma

$$\mathcal{R}_{\mathit{majority}}(Q) \leq 2\mathcal{R}_{\mathit{Gibbs}}(Q)$$

Observation:

$$h^Q_{\text{majority}}(x) = \operatorname{sign} \mathop{\mathbb{E}}_{h\sim Q} h(x) = \begin{cases} +1 & \text{if more than 50\% (probability mass) of the individual classifiers say } +1 \\ -1 & \text{otherwise} \end{cases}$$

$$\begin{aligned} \ell(y, h_{\text{majority}}(x)) = 1 \quad &\Rightarrow \quad \Pr_{h\sim Q}\{\ell(y, h(x)) = 1\} \geq 0.5 \\ \ell(y, h_{\text{majority}}(x)) = 1 \quad &\Rightarrow \quad 2 \mathop{\mathbb{E}}_{h\sim Q}[\ell(y, h(x))] \geq 1 \\ 2 \mathop{\mathbb{E}}_{h\sim Q}[\ell(y, h(x))] \quad &\geq \quad \ell(y, h_{\text{majority}}(x)) \\ 2\,\mathcal{R}_{\text{Gibbs}}(Q) \quad &\geq \quad \mathcal{R}_{\text{majority}}(Q) \end{aligned}$$

Generalization bounds for $\mathcal{R}_{\text{Gibbs}}$ also hold for $\mathcal{R}_{\text{majority}}$ (up to factor 2).

Example: Generalization bound for Gibbs classifier

Theorem (PAC-Bayesian generalization bound [McAllester, 1999])

Let the loss, ℓ, be a bounded in $[0,1]$. Let P be a "prior" distribution of $\mathcal{H}$, chosen independently of $\mathcal{D}$. With prob $1-\delta$ over $\mathcal{D} \overset{i.i.d.}{\sim} p^{\otimes n}$, it holds for all "posterior" distributions Q:

$$\mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}}\Big(KL(Q||P) + \frac{1}{8} + \log\frac{1}{\delta}\Big)$$

- Called PAC-Bayesian, because it makes a PAC-style statement (different between finite sample and expect error), but for Bayesian-style objects (distributions over classifiers/parameters)
- prior and posterior are in quotation marks, because the posterior is not the result of applying Bayes' rule.
- The prior is only a technical tool and shows up in the KL term. We don't have to "believe" in it or anything.

Towards a proof:

Theorem (Change of Measure Inequality)

For any distributions P, Q over $\mathcal{H}$ and function $\phi : \mathcal{H} \to \mathbb{R}$:

$$\mathop{\mathbb{E}}_{h\sim Q}[\phi(h)] \leq \frac{1}{\lambda}\Big(KL(Q||P) + \log \mathop{\mathbb{E}}_{h\sim P} e^{\lambda\phi(h)}\Big)$$

with $$KL(Q||P) = \mathop{\mathbb{E}}_{h\sim Q}\Big[\log \frac{Q(h)}{P(h)}\Big]$$

We shift from an expectation over P to an expectation over Q.

Very useful, e.g.

- P will be a typically a simple, data-independent, distribution
- Q will depend on a training set $\to$ "trained classifier"
- we "pay" for this: $\mathbb{E}_Q(\cdot)$ turns into $\log \mathbb{E}_P \exp(\cdot)$

Proof sketch, pretending P and Q have densities.

General observation:

$$\mathop{\mathbb{E}}_{h\sim P}[f(h)] = \int_{\mathcal{H}} P(h)f(h)dh = \int_{\mathcal{H}} Q(h)\frac{P(h)}{Q(h)}f(h)dh = \mathop{\mathbb{E}}_{h\sim Q}\left[\frac{P(h)}{Q(h)}f(h)\right]$$

$$\begin{aligned}
\log \mathop{\mathbb{E}}_{h\sim P}[e^{\lambda\phi(h)}] &= \log \mathop{\mathbb{E}}_{h\sim Q}\left[e^{\lambda\phi(h)}\frac{P(h)}{Q(h)}\right] \\
&\overset{\text{Jensen's ineq.}}{\geq} \mathop{\mathbb{E}}_{h\sim Q}\left[\log e^{\lambda\phi(h)}\frac{P(h)}{Q(h)}\right] \\
&= \mathop{\mathbb{E}}_{h\sim Q}\left[\lambda\phi(h) - \log\frac{Q(h)}{P(h)}\right] \\
&= \lambda \mathop{\mathbb{E}}_{h\sim Q}[\phi(h)] - \mathsf{KL}(Q||P)
\end{aligned}$$

$$\overset{\text{rearrange, } \cdot\frac{1}{\lambda}}{\Rightarrow} \quad \mathop{\mathbb{E}}_{h\sim Q}[\phi(h)] \leq \frac{1}{\lambda}\Big(\log \mathop{\mathbb{E}}_{h\sim P}[e^{\lambda\phi(h)}] + \mathsf{KL}(Q||P)\Big)$$

□

Theorem (Change of Measure Inequality)

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Theorem (PAC-Bayesian generalization bound [McAllester, 1999])

ℓ bounded in $[0,1]$. P independent of $\mathcal{D}$.

With prob $1-\delta$ over $\mathcal{D} \overset{i.i.d.}{\sim} p^{\otimes n}$, it holds for all distributions Q:

$$\mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}}\Big(KL(Q||P) + \frac{1}{8} + \log\frac{1}{\delta}\Big)$$

Proof sketch.

- Change of measure inequality:

$$\mathop{\mathbb{E}}_{h\sim Q}[\phi(h)] \leq \frac{1}{\lambda}\Big(\mathsf{KL}(Q||P) + \log \mathop{\mathbb{E}}_{h\sim P} e^{\lambda\phi(h)}\Big)$$

- apply with prior P, posterior Q and $\phi(h) = \mathcal{R}(h) - \hat{\mathcal{R}}(h)$:

$$\mathcal{R}(Q) - \hat{\mathcal{R}}(Q) \leq \frac{1}{\lambda}\Big(\mathsf{KL}(Q||P) + \log \mathop{\mathbb{E}}_{h\sim P} e^{\lambda[\mathcal{R}(h)-\hat{\mathcal{R}}(h)]}\Big)$$

- P and ϕ are independent (in contrast to Q), so with prob. $\geq 1-\delta$

$$\log \mathop{\mathbb{E}}_{h\sim P} e^{\lambda[\mathcal{R}(h)-\hat{\mathcal{R}}(h)]} \overset{\text{Hoeffing's lemma, Markov ineq.}}{\leq} \frac{\lambda^2 n}{8} + \log(1/\delta)$$

- theorem follows by setting $\lambda = \frac{1}{n}$.

□

Example: reproving a bound for finite hypothesis sets

- $\mathcal{H} = \{h_1, \ldots, h_T\}$ finite
- $P(h) = (\frac{1}{T}, \ldots, \frac{1}{T})$ uniform distribution
- $Q(h) = \delta_{h=h_k}(h)$ indicator on one hypothesis
- $\mathsf{KL}(Q||P) = \sum_t Q(t) \log \frac{Q(t)}{P(t)} = \log \frac{1}{P(h_k)} = \log T$

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The PAC-Bayesian statement for Gibbs classifiers:

$$\text{For every dist. } Q: \qquad \mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}}\left(\mathrm{KL}(Q||P) + \frac{1}{8} + \log\frac{1}{\delta}\right)$$

translates into a bound for a ordinary (deterministic) classifiers:

$$\text{For every } h \in \mathcal{H}: \qquad \mathcal{R}(h) \leq \hat{\mathcal{R}}(h) + \frac{1}{\sqrt{n}}\left(\log T + \frac{1}{8} + \log\frac{1}{\delta}\right)$$

which is similar to the previous bound for finite hypotheses sets.

Example: weighted finite hypothesis set bound

New: we can freely chose the prior, it does not have to be uniform.

- $\mathcal{H} = \{h_1, \ldots, h_T\}$ finite (or countable infinite)
- $P(h) = (\pi_1, \ldots, \pi_T)$ arbitrary prior distribution (fix before seeing $\mathcal{D}$)
- $Q(h) = \delta_{h=h_k}(h)$ indicator on one hypothesis
- $\mathrm{KL}(Q||P) = \sum_t Q(t) \log \frac{Q(t)}{P(t)} = \log \frac{1}{\pi_k}$

For every $h_k \in \mathcal{H}$:

$$\mathcal{R}(h_k) \leq \hat{\mathcal{R}}(h_k) + \frac{1}{\sqrt{n}}\left(\log \frac{1}{\pi_k} + \frac{1}{8} + \log \frac{1}{\delta}\right)$$

Better bound, if well-working hypotheses are (a priori) more likely.

Example: justifying L^2-regularization

- $\mathcal{H} = \{h_w(x) : \mathcal{X} \to \mathcal{Y},\ w \in \mathbb{R}^d\}$ parameterized by $w \in \mathbb{R}^d$
- $P(w) \propto e^{-\lambda \|w\|^2}$ prior: Gaussian around 0
- $Q(w) \propto e^{-\lambda \|w - v\|^2}$ posterior: Gaussian around v
- $\mathrm{KL}(Q||P) = \lambda \|v\|^2$

$$\mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}} \left(\lambda \|v\|^2 + \frac{1}{8} + \log \frac{1}{\delta} \right)$$

- most promising classifier: minimize right hand side w.r.t v
  $\to$ "regularizer" $\|v\|^2$ appears naturally in the objective

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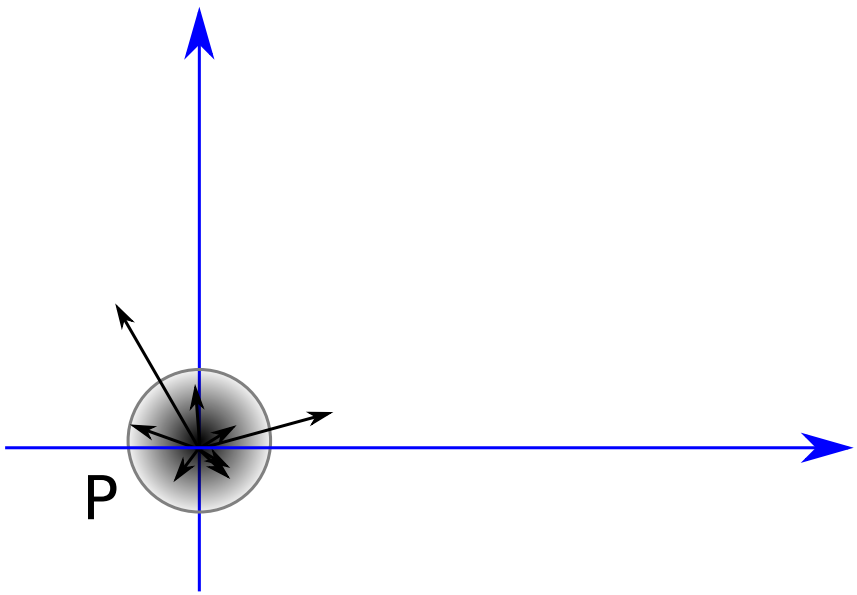
Caveat: $\|\cdot\|^2$ appears because we put it into the exponents of P and Q. Other distributions (which are our choice) yield other bounds/regularizers.

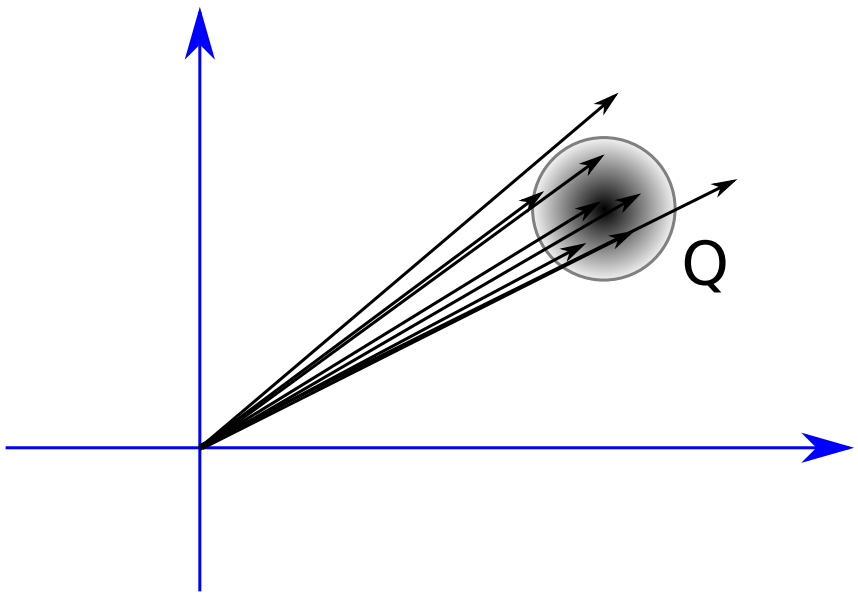
"PAC-Bayes is a bound-generation machine."

Example: SVM bound

- $\mathcal{H} = \{h(x) = \text{sign}\langle w, x\rangle,\ w \in \mathbb{R}^d\}$ linear classifiers
- $P(w) \propto e^{-\lambda\|w\|^2}$ prior: Gaussian around 0
- $Q(w) \propto e^{-\lambda\|w-v\|^2}$ posterior: Gaussian around v



prior: uniform w.r.t. direction



posterior: non-uniform

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- $P(w) \propto e^{-\lambda\|w\|^2}$ prior: Gaussian around 0
- $Q(w) \propto e^{-\lambda\|w-v\|^2}$ posterior shifted by v (non-uniform)

$$\mathcal{R}(Q) \le \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}}\Big(\lambda\|v\|^2 + \frac{1}{8} + \log\frac{1}{\delta}\Big)$$

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When ℓ is 0-1 loss:

- deterministic classifier $\text{sign}\langle v, x\rangle$ is identical to majority vote of Q
- we can relate $\hat{\mathcal{R}}(Q)$ to $\hat{\mathcal{R}}(v)$:

$$\hat{\mathcal{R}}(Q) = \frac{1}{n}\sum_{i=1}^{n} \bar{\Phi}\Big(\frac{y_i\langle v, x_i\rangle}{\|x_i\|}\Big) \text{ for } \bar{\Phi}(t) = \frac{1}{2}\Big(1 - \text{erf}\Big(\frac{t}{\sqrt{2}}\Big)\Big),$$

Together:

$$\frac{1}{2}\mathcal{R}(v) \le \frac{1}{n}\sum_{i=1}^{n} \bar{\Phi}\Big(\frac{y_i\langle v, x_i\rangle}{\|x_i\|}\Big) + \frac{\lambda}{\sqrt{n}}\|v\|^2 + \frac{\frac{1}{8} + \log\frac{1}{\delta}}{\sqrt{n}}$$

Example: Transfer bound

- $\mathcal{H} = \{h_w(x) : \mathcal{X} \to \mathcal{Y},\ w \in \mathbb{R}^d\}$ parameterized by $w \in \mathbb{R}^d$
- $P(w) \propto e^{-\lambda \|w - v_0\|^2}$ prior: Gaussian around v_0
- $Q(w) \propto e^{-\lambda \|w - v\|^2}$ posterior: Gaussian around v
- $\mathrm{KL}(Q||P) = \lambda \|v - v_0\|^2$

$$\mathcal{R}(Q) \leq \hat{\mathcal{R}}(Q) + \frac{1}{\sqrt{n}} \left(\lambda \|v - v_0\|^2 + \frac{1}{8} + \log \frac{1}{\delta} \right)$$

Typical situation for fine-tuning:

- inititalize classifier parameters as v_0
- train on $\mathcal{D}$ using (stochastic) gradient descent

Good generalization, if parameters don't move far from initialization.

"A PAC-Bayesian Tutorial with A Dropout Bound" [McAllester, 2013]

- "dropout rate" $\alpha \in [0, 1]$
- set of posterior distributions: $Q_{\theta,\alpha}$:

$$\text{for each weight:} \quad w_i = \begin{cases} 0 & \text{with prob. } \alpha \\ \theta_i + \epsilon_i & \text{otherwise, for } \epsilon_i \sim \mathcal{N}(0, 1) \end{cases}$$

- prior distribution: $P = Q_{0,\alpha}$
- $\mathrm{KL}(Q||P) = \frac{1-\alpha}{2}\|\theta\|^2$

Zero-ing out weights reduces complexity by factor $\frac{1-\alpha}{2}$:

$$\mathcal{R}(Q_{\theta,\alpha}) \leq \hat{\mathcal{R}}(Q_{\theta,\alpha}) + \frac{1}{\sqrt{n}}\Big(\frac{1-\alpha}{2}\|\theta\|^2 + \frac{1}{8} + \log\frac{1}{\delta}\Big)$$

Training: optimize $\hat{\mathcal{R}}(Q_{\theta,\alpha}) + \ldots$ via SGD $\rightarrow$ "dropout training"

Prediction: majority vote over many stochastic networks

Bounds for Deep Learning?

"Understanding deep learning requires rethinking generalization"

[Zhang, Bengio, Hardt, Recht, Vinyals, ICLR 2017]

Observation:

- Deep Neural Networks can have 100s of millions parameters.
- We train them with less than 1 million examples.
- Yet, they don't seem to overfit.
- Could it be that their capacity is much smaller than one would expect from the number of parameters?

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- let's explore their empirical Rademacher complexity
- train network with real input data, but random ± 1 labels

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Conclusion:

- we still don't know why deep networks don't overfit
- Rademacher-style learning theory does not explain it

"Stronger generalization bounds for deep nets via a compression approach"

[Arora, Ge, Neyshabur, Zhang. ICML 2018]

- $f : \mathcal{X} \to \mathcal{Y}$: trained network with many parameters
- $\mathcal{G}$: a set of (smaller) neural networks parametrized by q parameters, each of which can take r different values.

Theorem

Let $S = \{(x^1, y^1), \ldots, (x^m, y^m)\}$ be a training set with m samples. For $\lambda > 0$, if f can be approximated by a network $g \in \mathcal{G}$ in the sense that $|f(x^i) - g(x^i)| \leq \gamma$ for $i = 1, \ldots, m$, then (with high probability),

$$\mathcal{R}(g) \leq \frac{1}{m} \sum_{i=1}^{m} [\![y^i f(x^i) \leq \gamma]\!] + O\Big(\sqrt{\frac{q \log r}{m}}\Big)$$

Examples:

- quantize real-valued network parameter to a few (e.g. $r = 4$) bits
- low-rank decomposition of weight matrices to reduce number of coefficients

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Problem:

- theorem bounds quality of g, not f.
- the bound itself follows immediately from finite hypothesis set:
  - $\mathcal{R}(g) \leq \hat{\mathcal{R}}(g) + \sqrt{\frac{\log |\mathcal{G}| + \log 1/\delta}{m}}$ and $\log |\mathcal{G}| = \log r^q = q \log r$
  - $\hat{\mathcal{R}}(g) = \frac{1}{m} \sum_{i=1}^{m} [\![y^i g(x^i) \leq 0]\!] \leq \frac{1}{m} \sum_{i=1}^{m} [\![y^i f(x^i) \leq \gamma]\!]$

"Computing Nonvacuous Generalization Bounds for Deep (Stochastic) Neural Networks with Many More Parameters than Training Data" [Dziugaite, Roy. UAI 2016]

Observation:

- deep networks trained by SGD work well

Hypothesis:

- solution found by SGD are "shallow" minima of the objective, so it is robust against small perturbations of the network parameters

Approach:

- PAC-Bayesian bound:
  - prior: Gaussian around weight initialization w_0
  - posterior: Gaussian around learned parameters
- variance of Gaussians learned from bound itself (needs union bound)
- several approximations to approximate empirical risk

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Experiment (MNIST)	T-600	T-1200	T-300^2	T-600^2	T-1200^2	T-600^3	R-600
Test error	0.018	0.018	0.015	0.016	0.015	0.013	0.508
SNN test error	0.034	0.035	0.034	0.033	0.035	0.032	0.503
PAC-Bayes bound	0.161	0.179	0.170	0.186	0.223	0.201	1.352
VC dimension	26m	56m	26m	66m	187m	121m	26m

More...

"Spectrally-normalized margin bounds for neural networks"

[Bartlett, Foster Telgarsky, NIPS 2017]

Theorem 1.1. *Let nonlinearities $(\sigma_1, \ldots, \sigma_L)$ and reference matrices $(M_1, \ldots, M_L)$ be given as above (i.e., σ_i is ρ_i-Lipschitz and $\sigma_i(0) = 0$). Then for $(x, y), (x_1, y_1), \ldots, (x_n, y_n)$ drawn iid from any probability distribution over $\mathbb{R}^d \times \{1, \ldots, k\}$, with probability at least $1 - \delta$ over $((x_i, y_i))_{i=1}^n$, every margin $\gamma > 0$ and network $F_{\mathcal{A}} : \mathbb{R}^d \to \mathbb{R}^k$ with weight matrices $\mathcal{A} = (A_1, \ldots, A_L)$ satisfy*

$$\Pr\left[\arg\max_j F_{\mathcal{A}}(x)_j \neq y\right] \leq \widehat{\mathcal{R}}_\gamma(F_{\mathcal{A}}) + \widetilde{\mathcal{O}}\left(\frac{\|X\|_2 R_{\mathcal{A}}}{\gamma n}\ln(W) + \sqrt{\frac{\ln(1/\delta)}{n}}\right),$$

where $\widehat{\mathcal{R}}_\gamma(f) \leq n^{-1}\sum_i \mathbb{1}\left[f(x_i)_{y_i} \leq \gamma + \max_{j \neq y_i} f(x_i)_j\right]$ and $\|X\|_2 = \sqrt{\sum_i \|x_i\|_2^2}$.

"A PAC-Bayesian approach to spectrally-normalized margin bounds for neural networks" [Neyshabur, Bhojanapalli, Srebro, ICML 2018]

Theorem 1 (Generalization Bound)**.** *For any $B, d, h > 0$, let $f_{\mathbf{w}} : \mathcal{X}_{B,n} \to \mathbb{R}^k$ be a d-layer feedforward network with ReLU activations. Then, for any $\delta, \gamma > 0$, with probability $\geq 1 - \delta$ over a training set of size m, for any $\mathbf{w}$, we have:*

$$L_0(f_{\mathbf{w}}) \leq \widehat{L}_\gamma(f_{\mathbf{w}}) + \mathcal{O}\left(\sqrt{\frac{B^2 d^2 h \ln(dh) \Pi_{i=1}^d \|W_i\|_2^2 \sum_{i=1}^d \frac{\|W_i\|_F^2}{\|W_i\|_2^2} + \ln\frac{dm}{\delta}}{\gamma^2 m}}\right).$$