Computational Learning Theory

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Introduction

- For the analysis of data structures and algorithms and their limits we have:
  - **Computational complexity theory**
  - and analysis of **time** and **space** complexity
  - e.g. Dijkstra's algorithm or Bellman-Ford?
- For the analysis of ML algorithms, there are other questions we need to answer:
  - **Computational learning theory**
  - **Statistical learning theory**

Computational learning theory
(Wikipedia)

- **Probably approximately correct learning** (PAC learning) --Leslie Valiant
  - inspired boosting
- **VC theory** --Vladimir Vapnik
  - led to SVMs
- **Bayesian inference** --Thomas Bayes
- **Algorithmic learning theory** --E. M. Gold
- **Online machine learning** --Nick Littlestone

Today

- PAC model of learning
  - sample complexity,
  - computational complexity
- VC dimension
  - hypothesis space complexity
- SRM
  - model estimation
- examples throughout …

PAC learning

(L. Valiant, 1984)

- "Probably learning an approximately correct hypothesis"
- Problem setting:
  - learn an unknown target function c

$$c: X \rightarrow \{0,1\}, \qquad c \in C$$

  - given, training examples $\{x_i, c(x_i)\}$, of this target function
    - $x_i \in X$ i.i.d. according to an unknown but stationary distribution $\mathcal{D}$
  - given, a space of candidate hypothesis H

PAC learning: measures of error

- '**true error**' of hypothesis f w.r.t. target concept c, and instance distribution $\mathcal{D}$
$$\mathrm{error}_{\mathcal{D}}(f) = \Pr_{x\sim\mathcal{D}}[c(x) \neq f(x)]$$
  - the probability that f will misclassify an instance drawn at random according to $\mathcal{D}$
- '**training error**': $\mathrm{error}_{D}(f)$
  - fraction of training samples misclassified by f
  - this is the error that can be observed by our learner L

PAC-learnability: definition

- For concept class C to be PAC-learnable by L
  - we will require that error be bounded by some constant ϵ
  - and it's probability of failure be bounded by some constant δ

Definition: Consider a concept class C defined over a set of instances X of length n and a learner L using hypothesis space H. C is **PAC-learnable** by L using H if for all $c \in C$, distributions $\mathcal{D}$ over X, ϵ such that $0 < \epsilon < 1/2$, and δ such that $0 < \delta < 1/2$, learner L will with probability at least $(1 - \delta)$ output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \epsilon$, in time that is polynomial in $1/\epsilon$, $1/\delta$, n, and $size(c)$.

Sample complexity

- For finite hypothesis spaces $|H| < \infty$
  - for a consistent learner
  - for an agnostic learner
- For infinite hypothesis spaces
  - this is where VC dimension comes in

- Our analysis here is **worst-case**, because we demand that learner be general enough to learn any target concept $c \in C$ regardless of the distribution of training samples $\mathcal{D}$

Sample complexity: consistent finite $|H|$

- First a reminder of **version space**:
  - the set of all hypotheses that correctly classify the training samples

  $$VS_{H,D} = \{f \in H | (\forall \langle x, c(x) \rangle \in D)(f(x) = c(x))\}$$

- A **consistent learner** outputs a hypothesis belonging to VS
- To bound the number of samples needed by a consistent learner, it is enough to bound the number of samples needed to assure that VS contains no unacceptable f

Sample complexity: consistent finite $|H|$ (Haussler, 1988)

- The version space is **ϵ–exhausted** when all consistent hypotheses have true error less than ϵ
- So it bounds the probability that m training examples will fail to eliminate hypotheses with true error greater than ϵ

$$|H|e^{-\epsilon m}$$

Sample complexity: consistent finite $|H|$ (Haussler, 1988)

- Finally! we can determine the number of training samples required to reduce this probability below some desired δ

$$|H|e^{-\epsilon m} \leq \delta$$

$$m \geq \frac{1}{\epsilon}\left(\ln|H| + \ln\left({}^{1}/_{\delta}\right)\right)$$

- this number of training samples is enough to assure that any consistent hypothesis will be probably $(1-\delta)$ approximately (ϵ) correct

Sample complexity: inconsistent finite $|H|$

- What if H does not contain target concept c?
- We want learner to output $f \in H$ that has minimum training error
- Define f_{best} as the hypothesis from H with minimum training error
- How many training samples are needed to ensure that

$$\text{error}_{\mathcal{D}}(f_{\text{best}}) \leq \epsilon + \text{error}_{D}(f_{\text{best}})$$

Sample complexity: inconsistent finite $|H|$ (Hoeffding bounds, 1963)

- For a single hypothesis to have a misleading training error
  $$\Pr[\mathrm{error}_{\mathcal{D}}(f) > \epsilon + \mathrm{error}_{D}(f)\ ] \leq e^{-2m\epsilon^2}$$
- We want to assure that the best hypothesis has an error bounded this way
  - so consider that any one of them could have a large error
  $$\Pr[(\exists f \in H)\mathrm{error}_{\mathcal{D}}(f) > \epsilon + \mathrm{error}_{D}(f)\ ] \leq |H|e^{-2m\epsilon^2}$$

Sample complexity: inconsistent finite $|H|$ (Hoeffding bounds, 1963)

- So if do the stuff we did before, call that probability δ, we can find a bound for the number of samples needed to hold δ to some desired value

$$m \geq \frac{1}{2\epsilon^2}\left(\ln|H| + \ln\left({}^{1}/_{\delta}\right)\right)$$

Sample complexity: example

- C: conjunction of n boolean literals
- is C PAC-learnable?
- So $|H| = 3^n$ and

$$m \geq \frac{1}{\epsilon}\left(n \ln 3 + \ln({}^{1}/_{\delta})\right)$$

$$m = \frac{1}{.1}\left(10 \ln 3 + \ln({}^{1}/_{.05})\right) = 140$$

- m grows linearly in n, ϵ, and logarithmically in ${}^{1}/_{\delta}$
- So as long as L requires no more than polynomial computation per training sample, then total computation required will be polynomial as well.

Sample complexity: infinite $|H|$

- using $|H|$ leads to weak bounds
- and in case of $|H| = \infty$ we cannot apply it at all
- so we define a second measure of complexity called **VC dimension**
- in many cases it provides tighter bounds
- note (I will explain later):

$$\mathrm{VC}(H) \leq \log_2 |H|$$

VC theory

(V. Vapnik and A. Chervonenkis, 1960-1990)

- VC dimension
- Structural risk minimization

VC dimension

(V. Vapnik and A. Chervonenkis, 1968, 1971)

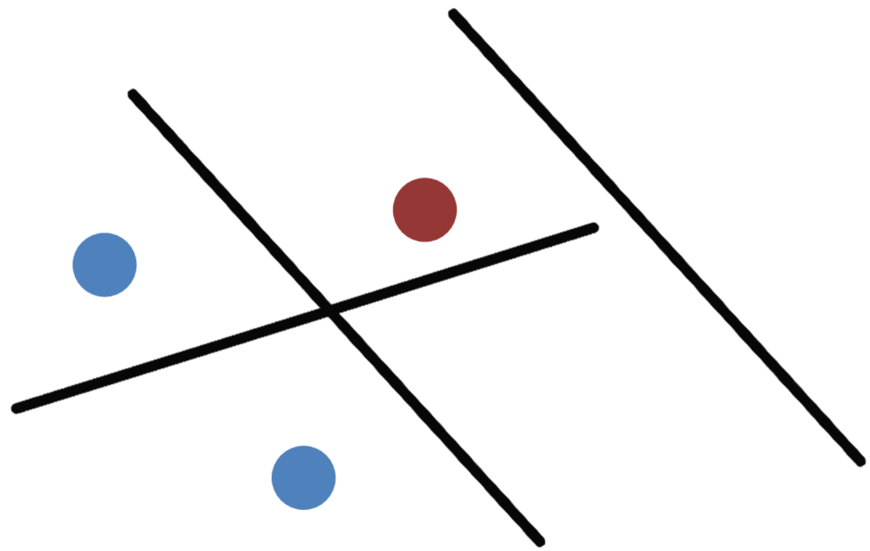
- First we'll define **shattering**
- Consider hypotheses for the two-class pattern recognition problem:

$$f(\mathbf{x}, \alpha) \in \{-1, 1\} \;\; \forall \mathbf{x}, \alpha$$

- Now, if for a set of N points that can be labeled in all 2^N ways (either $+$ or $-$),
  - a member of the set $\{f(\alpha)\}$ can be found which correctly assigns those labels…
  - we say, that set of points is **shattered** by $\{f(\alpha)\}$

VC dimension: example

three points in $\mathbb{R}^2$, shattered by oriented lines



- For our purposes, it is enough to find **one set of three points** that can be shattered
- It is not necessary to be able to shatter **every possible set of three points** in 2 dimensions

VC dimension: continued

- The **maximum number of points** that can be shattered by $H = \{f(\alpha)\}$ is called
  - **VC dimension of H**
  - and denoted as $\mathrm{VC}(H)$
- So the VC dimension of the set of oriented lines in $\mathbb{R}^2$ is three (last example)
- $\mathrm{VC}(H)$ is a measure of the **capacity** of the hypothesis class H
  - the higher the capacity, the higher the ability of the machine to learn any training set without error

VC dimension: intuition

- High capacity:
  - not a tree, b/c different from any tree I have seen (e.g. different number of leaves)
- Low capacity:
  - if it's green then it's a tree

Low VC dimension

- VC dimension is pessimistic
- If using **oriented lines** as our hypothesis class
  - we can only learn datasets with **3 points**!
- This is b/c VC dimension is computed independent of distribution of instances
  - In reality, near neighbors have same labels
  - So no need to worry about all possible labelings
- There are a lot of datasets containing more points that are learnable by a line!

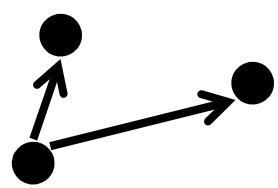
Infinite VC dimension

- Lookup table has infinite VC dimension
- But so does the nearest neighbor classifier
  – b/c any number of points, labeled arbitrarily (w/o overlaps), will be successfully learned
- But it performs well…

- So infinite capacity **does not guarantee** poor generalization performance

Examples of calculating VC dimension

- So we saw that the VC dimension of the set of oriented lines in $\mathbb{R}^2$ is 3
- Generally, the VC dimension of the set of oriented hyperplanes in $\mathbb{R}^n$ is $n + 1$



Examples of calculating VC dimension: continued

- Let K be a positive kernel which corresponds to a minimal embedding space $\mathcal{H}$.
- Then the VC dimension of the corresponding support vector machine is $\dim(\mathcal{H}) + 1$.
- Proof…

VC dimension of SVMs with polynomial kernels

- e.g. $k(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle^2$
- if $\mathbf{x}$ and $\mathbf{y}$ are 2-dimensional:

$$k(\mathbf{x}, \mathbf{y}) = (x_1 y_1 + x_2 y_2)^2 = x^2 y^2 + 2 x_1 y_1 x_2 y_2 + x^2 y^2$$

  - the feature space is 3-dimensional
  - and the VC dimension of an SVM with this kernel is $3 + 1 = 4$
- in general, for a space with dimension d, the dimension of the embedding space for homogeneous polynomial kernels is

$$\binom{d + p - 1}{p}$$

Sample complexity and the VC dimension
(Blumer et al., 1989)

$$m \geq \frac{1}{\epsilon}\left(4\log_2\left({}^{2}/_{\delta}\right) + 8h\log_2\left({}^{13}/_{\epsilon}\right)\right)$$

- where $h = \mathrm{VC}(H)$

Structural risk minimization

(V. Vapnik and A. Chervonenkis, 1974)

- A function that fits training data and minimizes VC dimension
  - will **generalize well**
- SRM provides a quantitative characterization of the **tradeoff** between
  - the complexity of the approximating functions,
  - and the quality of fitting the training data
- First, we will talk about a certain bound..

A bound

- on the generalization performance of a pattern recognition learning machine
  - from Burges, 1998

true mean error/ actual risk

$$R(\alpha) = \int \frac{1}{2} |y - f(\mathbf{x}, \alpha)| dP(\mathbf{x}, y)$$

$$R(\alpha) = \int \frac{1}{2} |y - f(\mathbf{x}, \alpha)| p(\mathbf{x}, y) d\mathbf{x} dy$$

$$R_{emp}(\alpha) = \frac{1}{2N} \sum_{i=1}^{N} |y_i - f(\mathbf{x}_i, \alpha)|$$

empirical risk

A bound: continued

VC confidence

$$R(\alpha) \leq R_{emp}(\alpha) + \sqrt{\left(\frac{h(\log(2N/h)+1) - \log(\eta/4)}{N}\right)}$$

risk bound

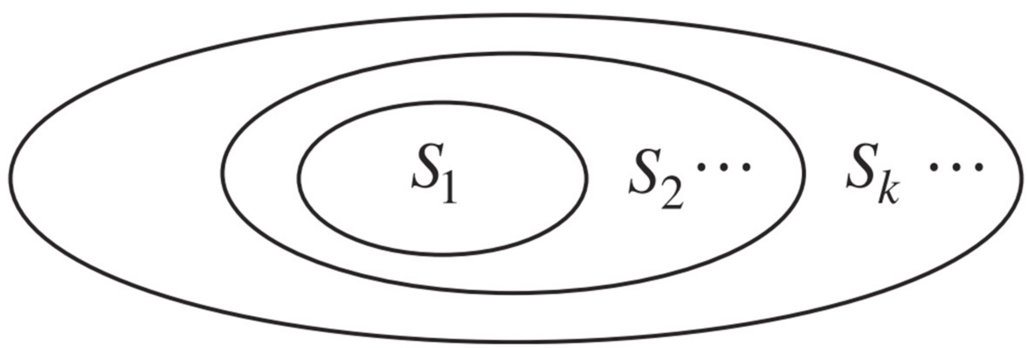
SRM: continued

- To minimize true error (actual risk), both empirical risk and VC confidence term should be minimized
- The VC confidence term depends on the chosen **class of functions**
- Whereas empirical risk and actual risk depend on the **one particular function** chosen for training

SRM: continued

- The VC dimension h doesn't vary smoothly since it is an integer
- Therefore the entire class of functions is structured into nested subsets (ordered by $h, h < \infty$)

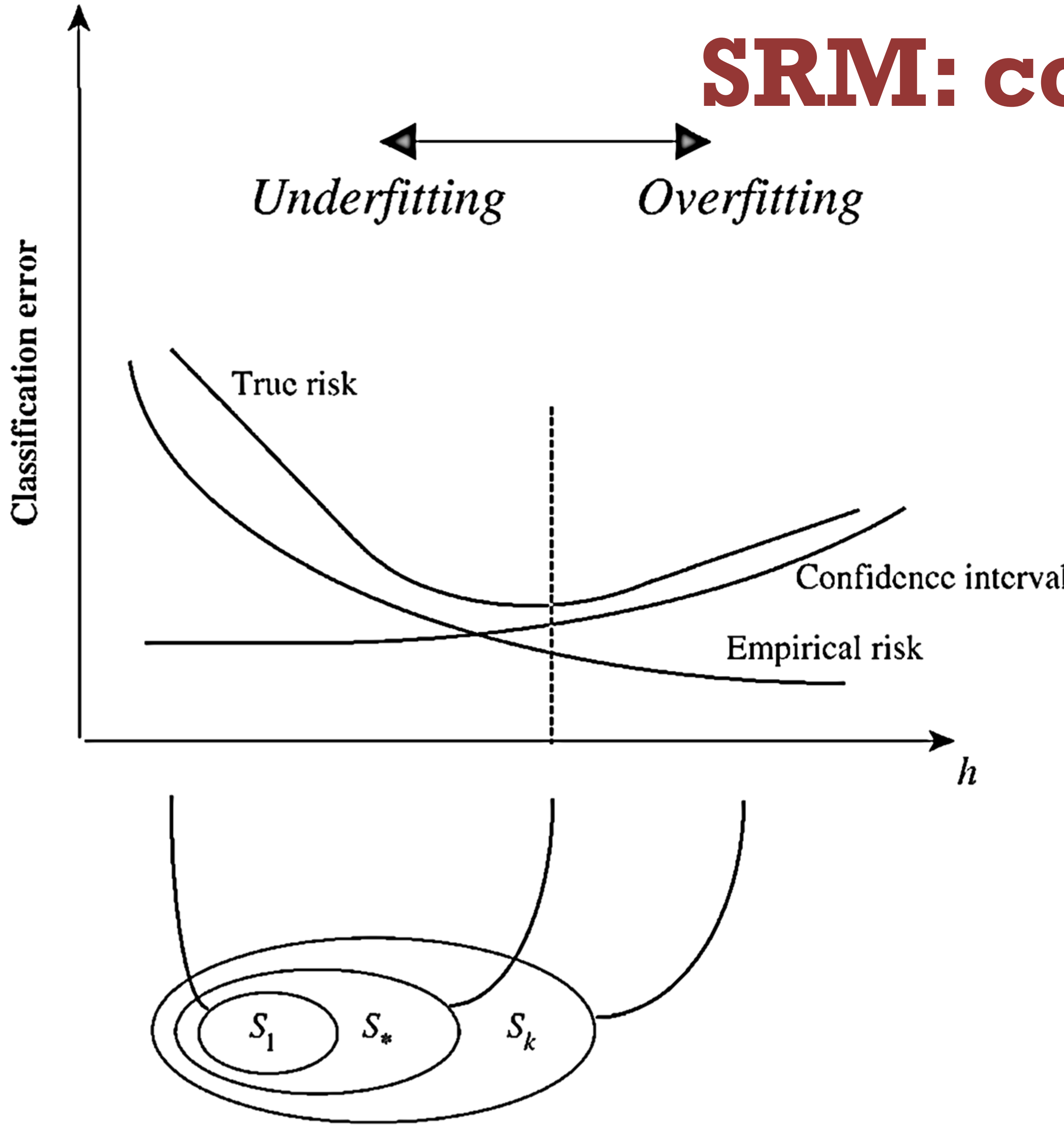
$$h_1 \leq h_2 \leq \cdots \leq h_k \leq \cdots.$$



SRM: continued

- For a given data set, optimal model estimation with SRM consists of the following steps:
  1. select an element of a structure (model selection)
  2. estimate the model from this element (statistical parameter estimation)

SRM: continued



SRM chooses the subset S_i for which minimizing the empirical risk yields the best bound on the true risk.

Support vector machine

(Vapnik, 1982)

- Does SVM implement the SRM principle?
- We have shown that the VC dimension of a nonlinear SVM is $\dim(\mathcal{H}) + 1$, where $\dim(\mathcal{H})$ is the dimension of space $\mathcal{H}$
- and equal to $\binom{d_L + p - 1}{p}$ and ∞ for a –degree polynomial and RBF kernel, respectively
  – So SVM can have very high VC dimension
- But, it is possible to prove that SVM training actually minimizes the VC dimension and empirical error at the same time.

Support vector machine

(Vapnik, 1995)

- Given m data points in $\mathbb{R}^n$, $\|x_i\| \leq R$
- H_γ: set of linear classifiers in $\mathbb{R}^n$ with margin γ on X
- Then

$$\mathrm{VC}(H) \leq \min\left\{n, \left\lceil \frac{4R^2}{\gamma^2} \right\rceil\right\}$$

- This means that hypothesis spaces with large margin have small VC dimension
- (Burges, 1998) claimed that this bound is for a gap-tolerant classifier but not the SVM classifier…

What we said today

- PAC bounds
  - only apply to finite hypothesis spaces
- VC dimension is a measure of complexity
  - can be applied for infinite hypothesis spaces
- Training neural networks uses only ERM, whereas SVMs use SRM
- Large margins imply small VC dimension ☺

References

1. Machine Learning by T. M. Mitchell
2. A Tutorial on Support Vector Machines for Pattern Recognition by C. J. C. Burges
3. http://www.svms.org/

Thanks!
Questions?