Carnegie Mellon University
School of Computer Science

10701: Introduction to Machine Learning

Computational Learning Theory II:
VC Dimension and Model Complexity

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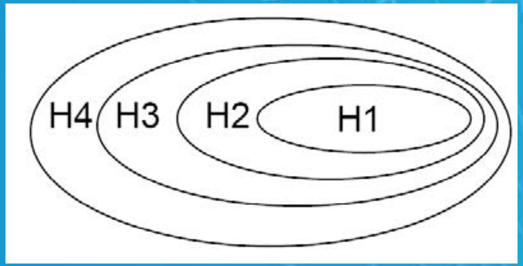
Reading: Chap. 7 T.M book, and outline material



Last time: PAC and Agnostic Learning

- Finite H, assume target function c ∈ H

$$Pr(\exists h \in H,\ s.t.\ (error_{train}(h) = 0) \wedge (error_{true}(h) > \epsilon)\ ) \leq |H| e^{-\epsilon m}$$

  - Suppose we want this to be at most δ. Then *m* examples suffice:

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

- Finite H, agnostic learning: perhaps c *not* in H

$$P(\exists h \in H,\ |\epsilon(h) - \hat{\epsilon}(h)| > \gamma) \quad = \quad 2k \exp(-2\gamma^2 m)$$

  - ➔ $$m \geq \frac{1}{2\gamma^2} \log \frac{2k}{\delta}$$
  - with probability at least (1-δ) every h in H satisfies

$$\epsilon(\hat{h}) \leq \left(\min_{h \in H} \epsilon(h)\right) + 2\sqrt{\frac{1}{m} \log \frac{2k}{\delta}}$$

What if H is not finite?

- Can't use our result for infinite H

- Need some other measure of complexity for H
  – Vapnik-Chervonenkis (VC) dimension!

What if H is not finite?

- Some Informal Derivation
  - Suppose we have an H that is parameterized by d real numbers. Since we are using a computer to represent real numbers, and IEEE double-precision floating point (double's in C) uses 64 bits to represent a floating point number, this means that our learning algorithm, assuming we're using double-precision floating point, is parameterized by 64d bits

- Parameterization

How do we characterize "power"?

- Different machines have different amounts of "power".
- Tradeoff between:
  - More power: Can model more complex classifiers but might overfit.
  - Less power: Not going to overfit, but restricted in what it can model

- How do we characterize the amount of power?

Shattering a Set of Instances

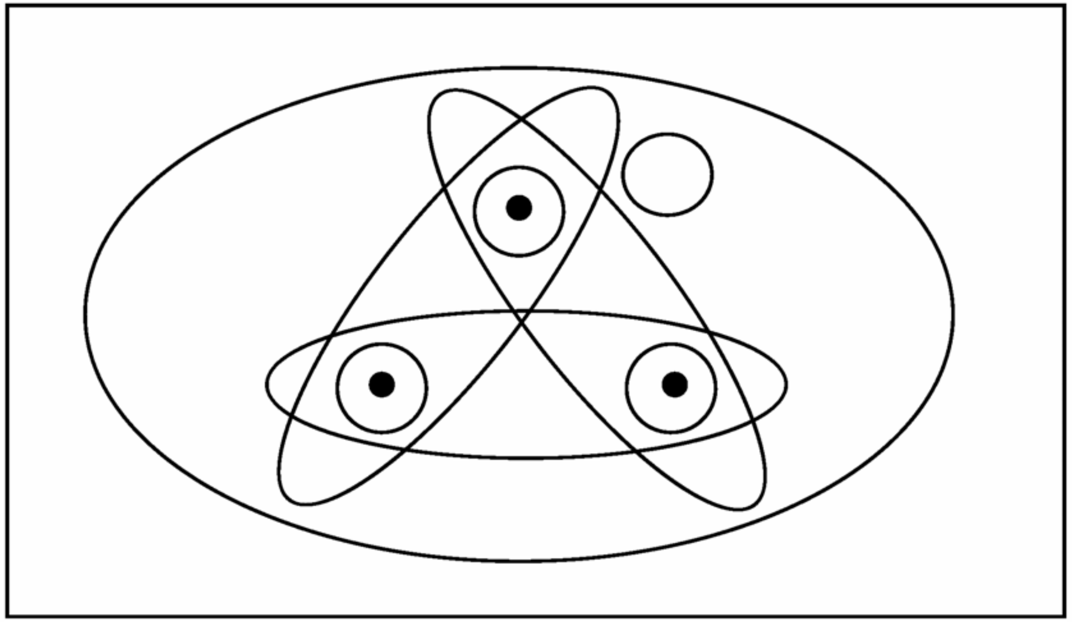
- *Definition*: Given a set $S = \{x^{(1)}, \dots, x^{(m)}\}$ (no relation to the training set) of points $x^{(i)} \in X$, we say that H shatters S if H can realize any labeling on S.

  I.e., if for any set of labels $\{y^{(1)}, \dots, y^{(d)}\}$, there exists some $h \in H$ so that $h(x^{(i)}) = y^{(i)}$ for all $i = 1, \dots, m$.

- There are 2^m different ways to separate the sample into two sub-samples (a dichotomy)

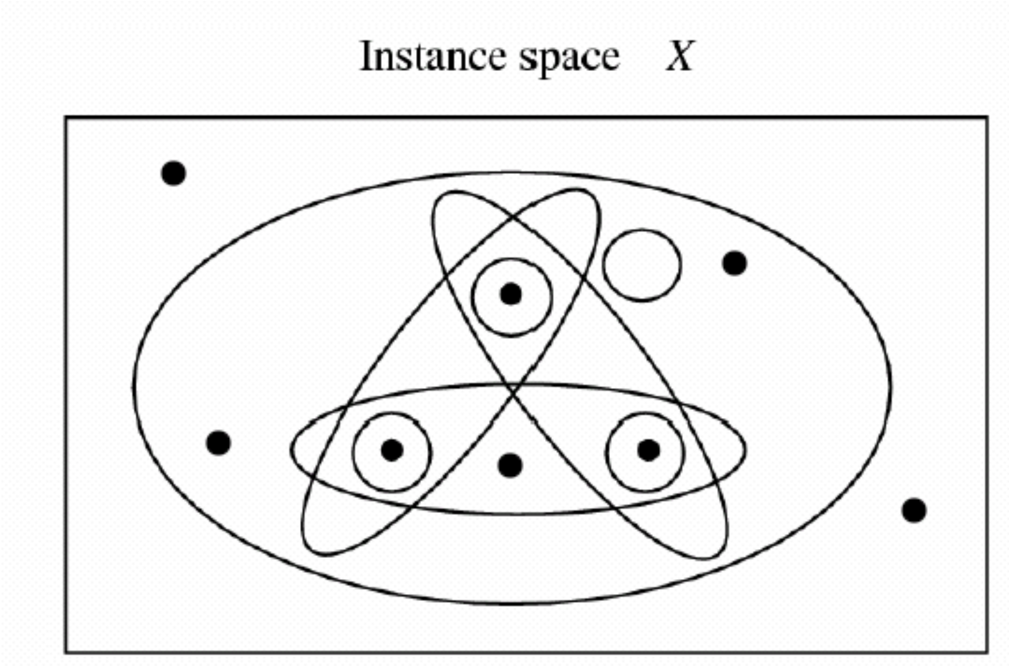
Three Instances Shattered

Instance space X



The Vapnik-Chervonenkis Dimension

- *Definition*: The **Vapnik-Chervonenkis dimension**, $VC(H)$, of hypothesis space H defined over instance space X is the size of the *largest finite subset* of X shattered by H. If arbitrarily large finite sets of X can be shattered by H, then $VC(H) \equiv \infty$.



VC dimension: examples

Consider $X = \mathbb{R}$, want to learn $c: X \rightarrow \{0,1\}$

What is VC dimension of

- Open intervals:

  H1: if $x>a$, then $y=1$ else $y=0$

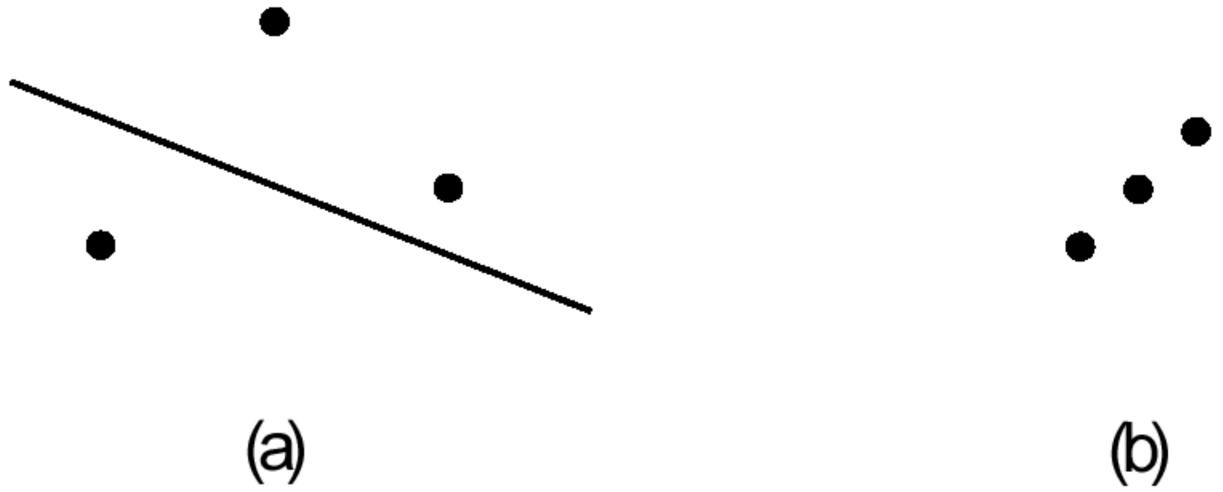
- Closed intervals:

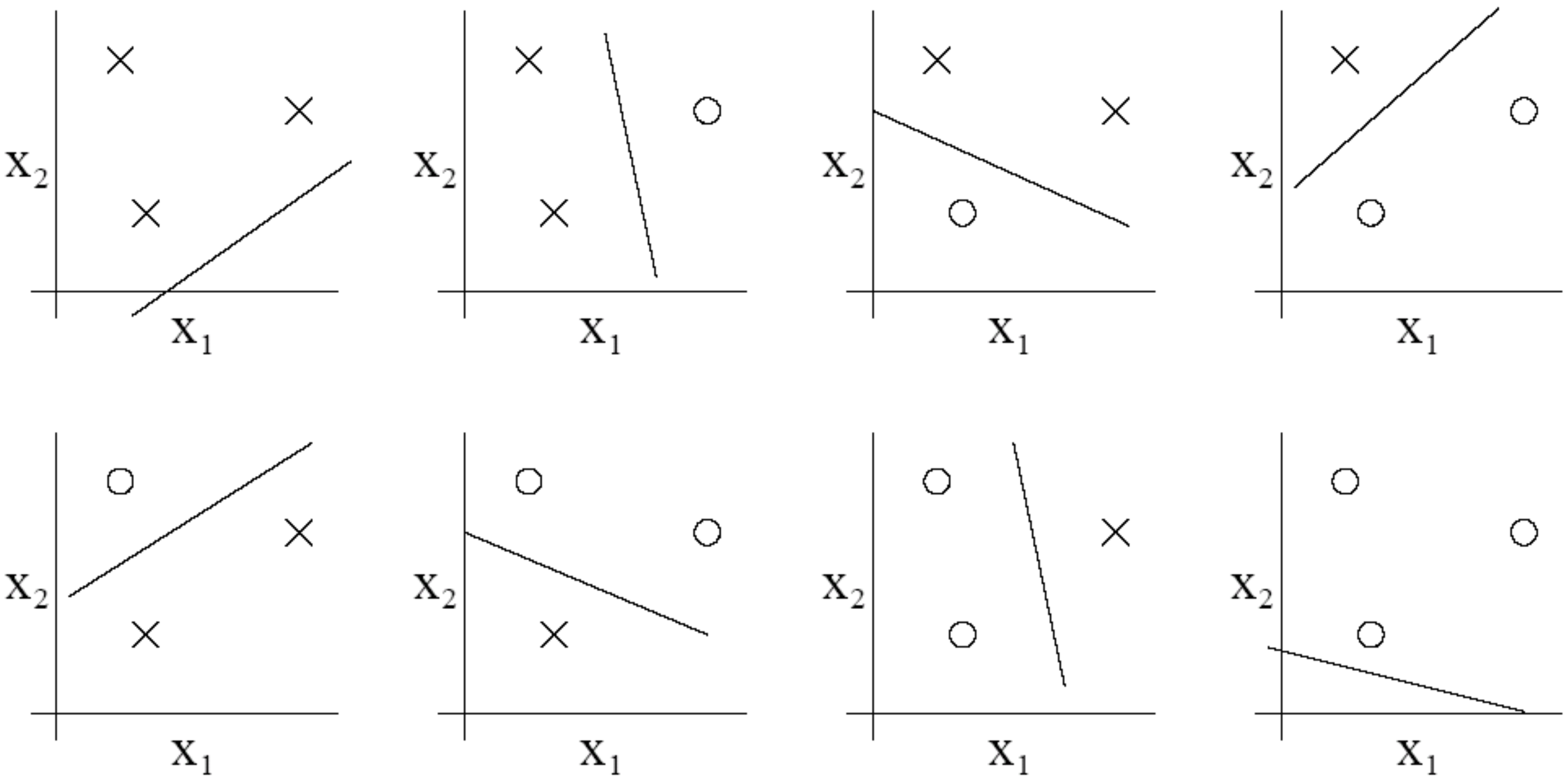
  H2: if $a<x<b$, then $y=1$ else $y=0$

VC dimension: examples

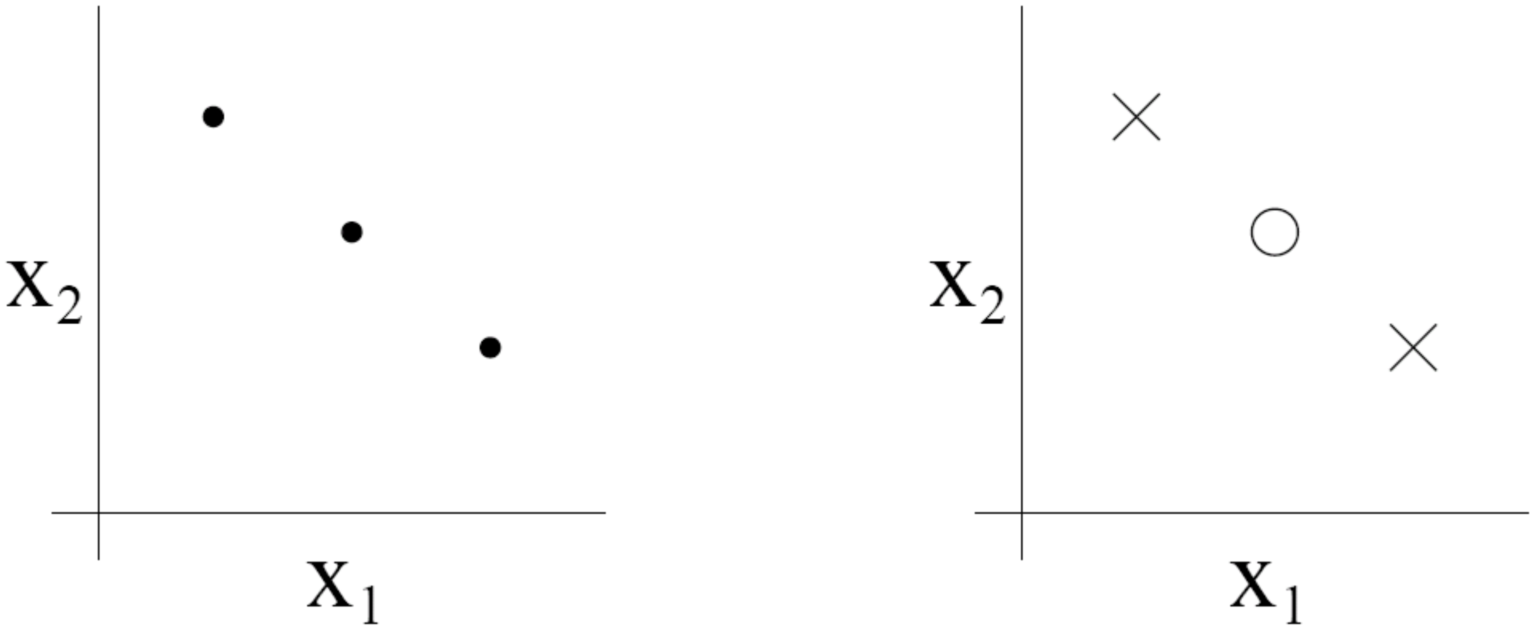
Consider X = $\mathbb{R}^2$, want to learn c: X→{0,1}

- What is VC dimension of lines in a plane?
  H= { ((wx+b)>0 → y=1) }





- For any of the eight possible labelings of these points, we can find a linear classier that obtains "zero training error" on them.
- Moreover, it is possible to show that there is no set of 4 points that this hypothesis class can shatter.



- The VC dimension of H here is 3 even though there may be sets of size 3 that it cannot shatter.
- under the definition of the VC dimension, in order to prove that VC(H) is at least *d*, we need to show only that there's at least one set of size d that H can shatter.

- **Theorem** Consider some set of m points in $\mathbf{R}^n$. Choose any one of the points as origin. Then the m points can be shattered by oriented hyperplanes if and only if the position vectors of the remaining points are linearly independent.

- **Corollary**: The VC dimension of the set of oriented hyperplanes in $\mathbf{R}^n$ is n+1.

  Proof: we can always choose $n + 1$ points, and then choose one of the points as origin, such that the position vectors of the remaining n points are linearly independent, but can never choose $n + 2$ such points (since no $n + 1$ vectors in $\mathbf{R}^n$ can be linearly independent).

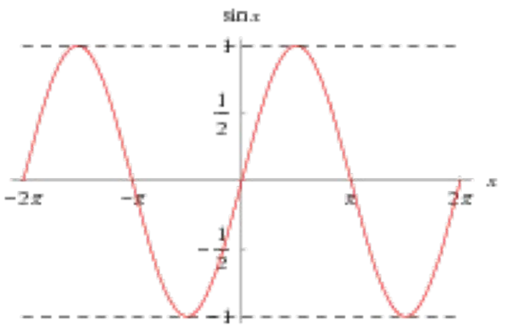
The VC Dimension and the Number of Parameters

- The VC dimension thus gives concreteness to the notion of the capacity of a given set of *h*.
- Is it true that learning machines with many parameters would have high VC dimension, while learning machines with few parameters would have low VC dimension?

An infinite-VC function with just one parameter!

$$f(x, \alpha) \equiv \theta(\sin(\alpha x)), \quad x, \alpha \in R$$

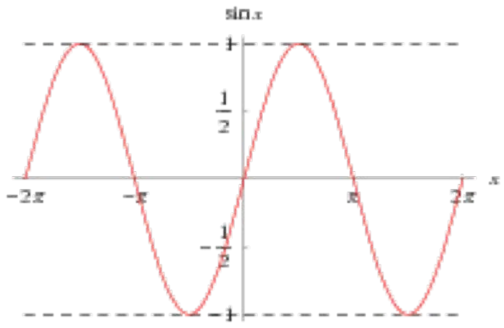
where θ is an indicator function



An infinite-VC function with just one parameter

- You choose some number l, and present me with the task of finding l points that can be shattered. I choose them to be

$$x_i = 10^{-i} \quad i = 1, \ldots, l.$$



- You specify any labels you like:

$$y_1, y_2, \ldots, y_l, \quad y_i \in \{-1, 1\}$$

- Then $\theta(\alpha)$ gives this labeling if I choose α to be

$$\alpha = \pi(1 + \sum_{i=1}^{l} \frac{(1 - y_i)10^i}{2})$$

- Thus the VC dimension of this machine is infinite.

Sample Complexity from VC Dimension

- How many randomly drawn examples suffice to ε-exhaust $VS_{H,S}$ with probability at least (1 - δ)?

  ie., to guarantee that any hypothesis that perfectly fits the training data is probably (1-δ) approximately (ε) correct on testing data from the same distribution

$$m \geq \frac{1}{\varepsilon}\left(4\log_2(2/\delta) + 8VC(H)\log_2(13/\varepsilon)\right)$$

Compare to our earlier results based on $|H|$:

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

Mistake Bounds

So far: how many examples needed to learn?

What about: how many mistakes before convergence?

Let's consider similar setting to PAC learning:

- Instances drawn at random from X according to distribution D
- Learner must classify each instance before receiving correct classification from teacher
- Can we bound the number of mistakes learner makes before converging?

Statistical Learning Problem

- A model computes a function: $h(X,w)$
- Problem : minimize in w Risk Expectation

$$R(w) = \int Q(z,w)dP(z)$$

- w : a parameter that specifies the chosen model
- $z = (X, y)$ are possible values for attributes (variables)
- Q measures (quantifies) model error cost
- $P(z)$ is the underlying probability law (unknown) for data z

Statistical Learning Problem (2)

- We get m data from learning sample $(z_1, .. , z_m)$, and we suppose them iid sampled from law $P(z)$.
- To minimize $R(w)$, we start by minimizing Empirical Risk over this sample :

$$E(W) = \frac{1}{m} \sum_{i=1}^{m} Q(Z_i, W)$$

- We shall use such an approach for :
  - classification (eg. Q can be a cost function based on cost for misclassified points)
  - regression (eg. Q can be a cost of least squares type)

Statistical Learning Problem (3)

- Central problem for Statistical Learning Theory:

  What is the relation
  between Risk Expectation $R(W)$
  and Empirical Risk $E(W)$?

- How to define and measure a generalization capacity ("robustness") for a model ?

Four Pillars for SLT

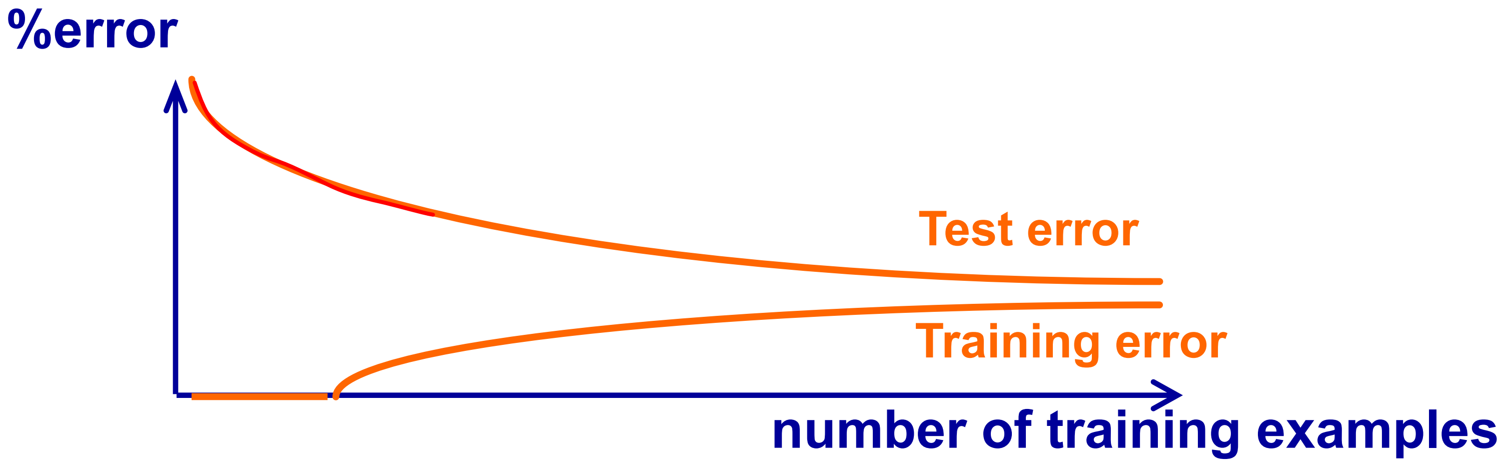
- Consistency (guarantees generalization)
  - Under what conditions will a model be consistent ?

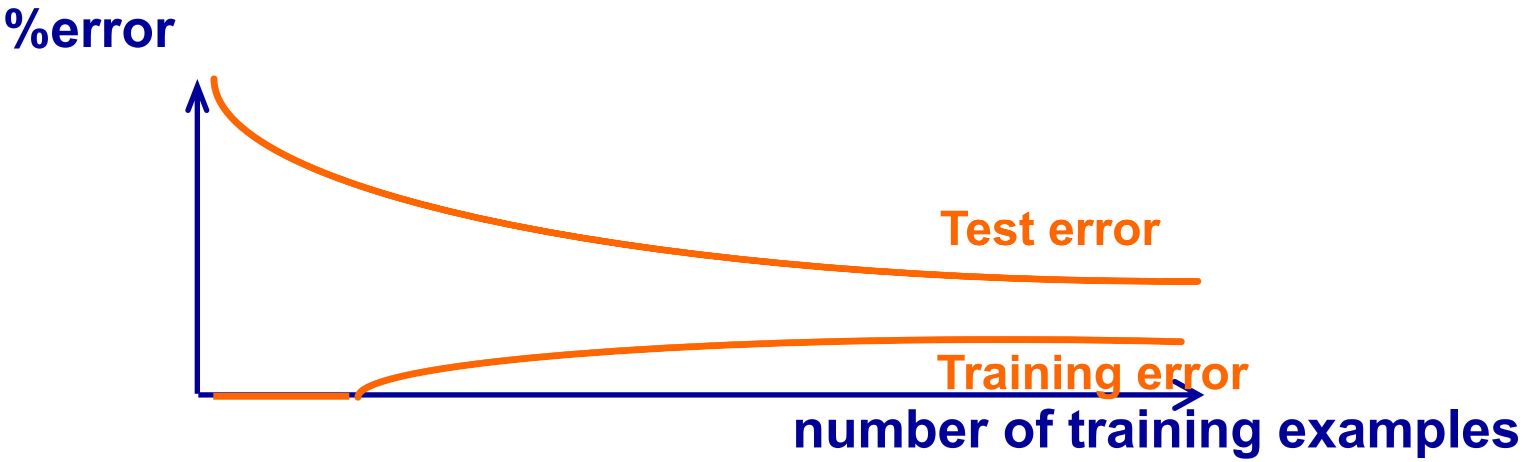
- Model convergence speed (a measure for generalization)
  - How does generalization capacity improve when sample size L grows?

- Generalization capacity control
  - How to control in an efficient way model generalization starting with the only given information we have: our sample data?

- A strategy for good learning algorithms
  - Is there a strategy that guarantees, measures and controls our learning model generalization capacity ?

Consistent training?





Vapnik main theorem

- Q : Under which conditions will a learning model be consistent?
- A : A model will be consistent if and only if the function h that defines the model comes from a family of functions H with finite VC dimension d

- A finite VC dimension d not only guarantees a generalization capacity (consistency), but to pick h in a family H with finite VC dimension d is the only way to build a model that generalizes.

Model convergence speed (generalization capacity)

- Q : What is the nature of model error difference between learning data (sample) and test data, for a sample of finite size *m*?
- A : This difference is no greater than a limit that only depends on the ratio between VC dimension *d* of model functions family *H*, and sample size *m*, i.e., *d/m*

This statement is a new theorem that belongs to Kolmogorov-Smirnov way for results, i.e., theorems that do not depend on data's underlying probability law.

Agnostic Learning: VC Bounds

- *Theorem*: Let H be given, and let d = VC(H). Then with probability at least 1-δ , we have that for all h $\in$ H,

$$|\hat{\epsilon}(h) - \epsilon(h)| \leq O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} - \frac{1}{m}\log\delta}\right)$$

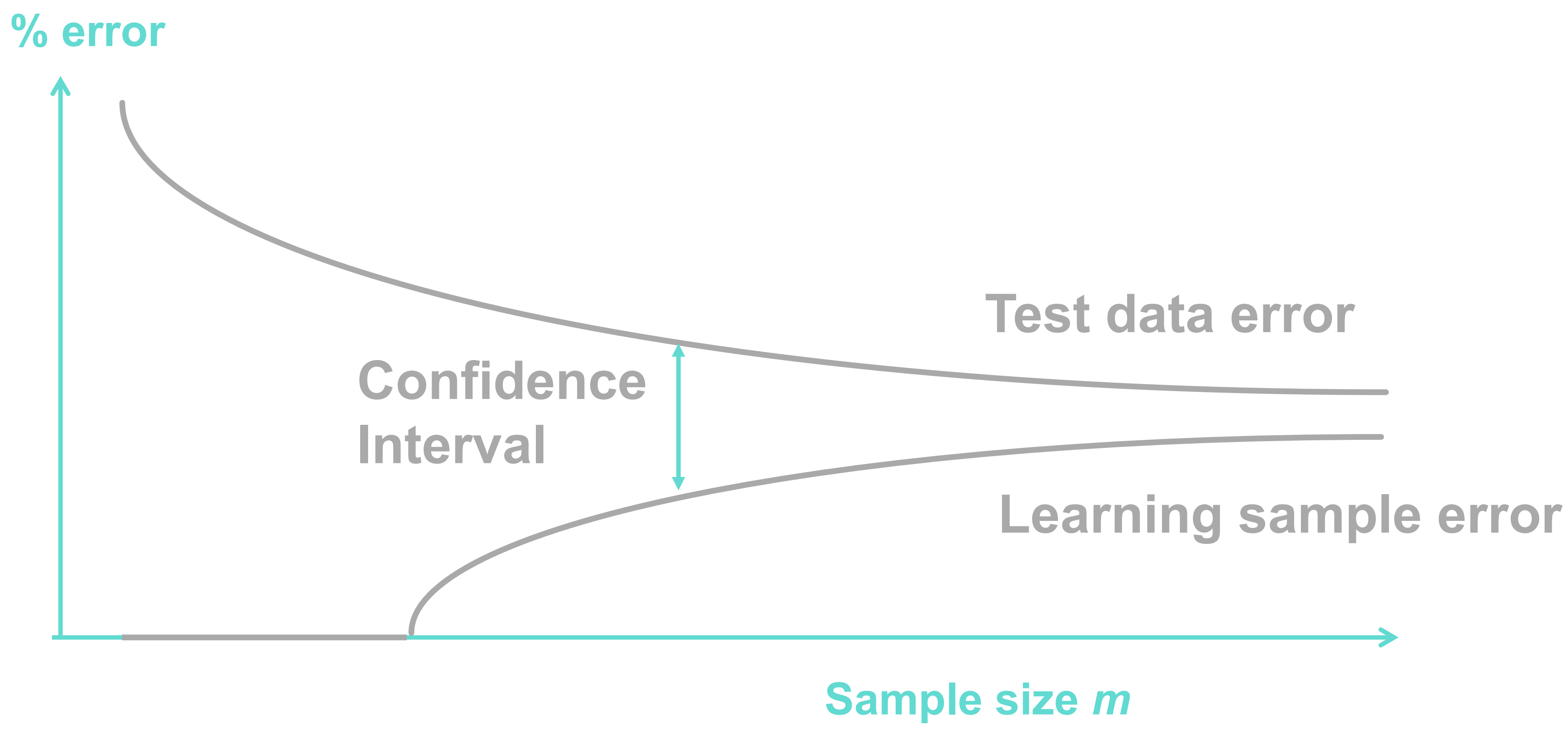
or

$$\epsilon(h) \leq \hat{\epsilon}(h) + O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} - \frac{1}{m}\log\delta}\right)$$

recall that in finite H case, we have:

$$|\hat{\epsilon}(h) - \epsilon(h)| \leq \sqrt{\frac{1}{m}\log 2k - \frac{1}{m}\log\delta}$$

Model convergence speed



How to control model generalization capacity

Risk Expectation = Empirical Risk + Confidence Interval

- To minimize Empirical Risk alone will not always give a good generalization capacity: one will want to minimize the sum of Empirical Risk and Confidence Interval

- What is important is not the numerical value of the Vapnik limit, most often too large to be of any practical use, it is the fact that this limit is a non decreasing function of model family function “richness”

Empirical Risk Minimization

- With probability $1-\delta$, the following inequality is true:

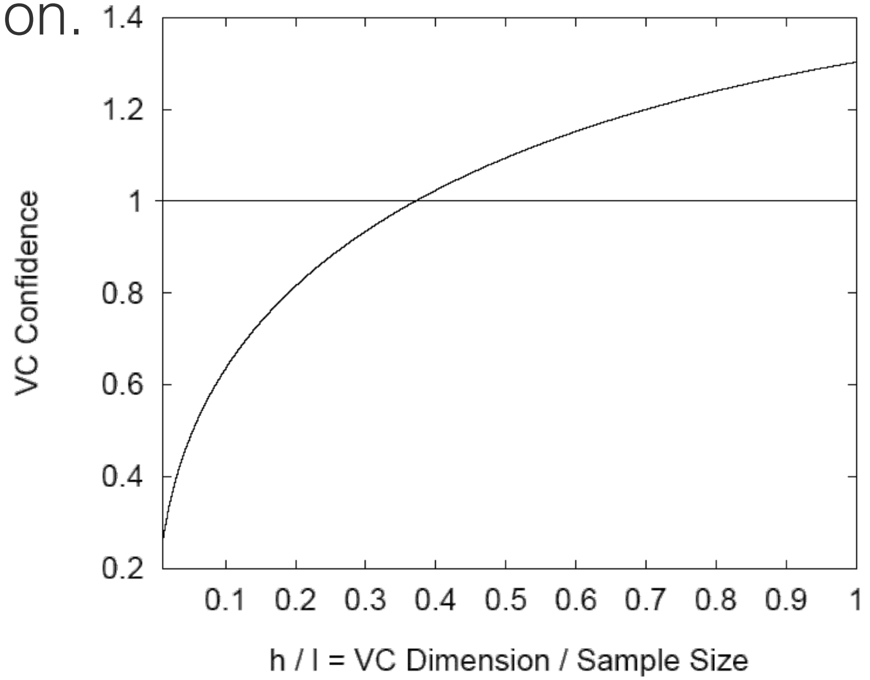
$$\int \left(y - f(x, w^0)\right)^2 dP(x,y) < \frac{1}{m}\sum_{i=1}^{m}\left(y_i - f(x_i, w^0)\right)^2 + \sqrt{\frac{d\left(\ln\left(2m/d\right)+1\right) - \ln\delta}{m}}$$

- where w^0 is the parameter w value that minimizes Empirical Risk:

$$E(W) = \frac{1}{m}\sum_{i=1}^{m}\left(y_i - f(x_i, w)\right)^2$$

Minimizing The Bound by Minimizing *d*

- Given some selection of learning machines whose empirical risk is zero, one wants to choose that learning machine whose associated set of functions has minimal VC dimension.

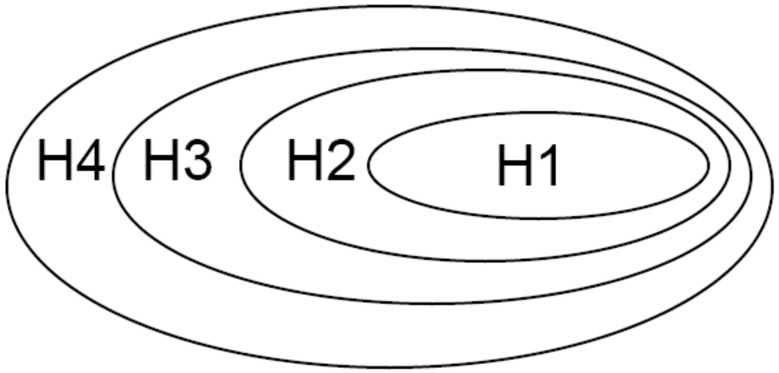


  - By doing this we can attain an upper bound on the actual risk. This does not prevent a particular machine with the same value for empirical risk, and whose function set has higher VC dimension, from having better performance.
  - What is the VC of a kNN?

Structural Risk Minimization

- Which hypothesis space should we choose?

- Bias / variance tradeoff



- SRM: choose H to minimize bound on true error!

$$\epsilon(h) \leq \hat{\epsilon}(h) + O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} - \frac{1}{m}\log\delta}\right)$$

unfortunately a somewhat loose bound...

SRM strategy (1)

- With probability $1\text{-}\delta$,

$$\epsilon(h) \leq \hat{\epsilon}(h) + O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} - \frac{1}{m}\log\delta}\right)$$

- When m/d is small (d too large), second term of equation becomes large
- SRM basic idea for strategy is to minimize simultaneously both terms standing on the right of above majoring equation for $\varepsilon(h)$
- To do this, one has to make d a controlled parameter

SRM strategy (2)

- Let us consider a sequence $H_1 < H_2 < .. < H_n$ of model family functions, with respective growing VC dimensions

  $d_1 < d_2 < .. < d_n$

- For each family H_i of our sequence, the inequality

$$\epsilon(h) \leq \hat{\epsilon}(h) + O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} - \frac{1}{m}\log\delta}\right)$$

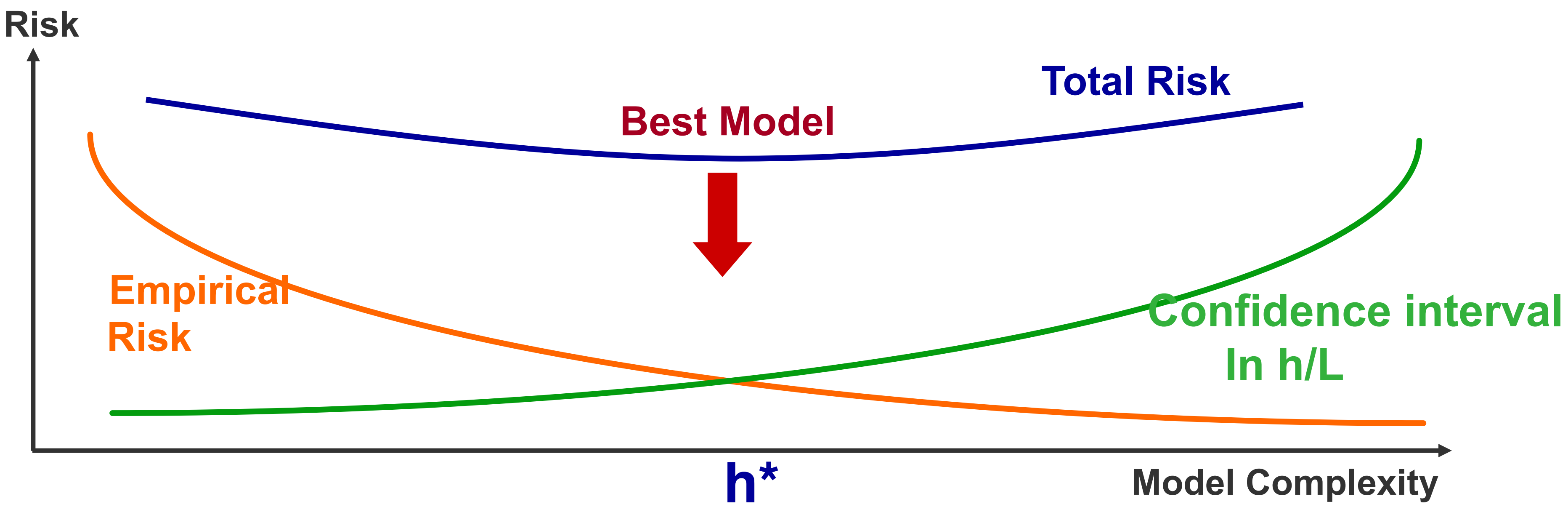
  is valid

  - That is, for each subset, we must be able either to compute d, or to get a bound on d itself.

- SRM then consists of finding that subset of functions which minimizes the bound on the actual risk.

SRM strategy (3)

SRM : find i such that expected risk $\varepsilon(h)$ becomes minimum, for a specific $d^*=d_i$, relating to a specific family H_i of our sequence; build model using h from H_i



Putting SRM into action: linear models case (1)

- There are many SRM-based strategies to build models:

- In the case of linear models

  $y = \langle w|x \rangle + b,$

  one wants to make $||w||$ a controlled parameter: let us call H_C the linear model function family satisfying the constraint:

  $||w|| < C$

> Vapnik Major theorem:
>
> When C decreases, $d(H_C)$ decreases
>
> $||x|| < R$

Putting SRM into action: linear models case (2)

- To control ||w||, one can envision two routes to model:
  - *Regularization/Ridge Regression, ie min. over w and b*

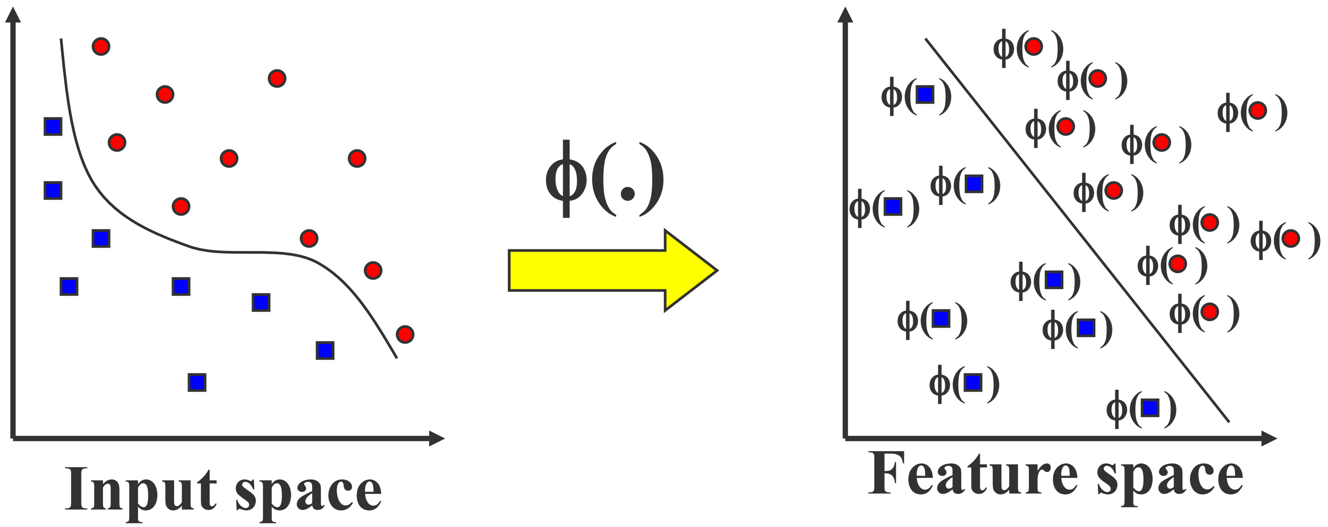
    $$RG(w,b) = S\{(y_i - \langle w|x_i\rangle - b)^2 \,|\, i=1,..,L\} + \lambda \,||w||^2$$

  - *Support Vector Machines (SVM), ie solve directly an optimization problem (classif. SVM, separable data)*

    Minimize $||w||^2$,
    with $(y_i = +/-1)$
    and $y_i(\langle w|x_i\rangle + b) >= 1$ *for all* $i=1,..,L$

The VC Dimension of SVMs

- An SVM finds a linear separator in a Hilbert space, where the original date x can be mapped to via a transformation $\phi(x)$.



- Recall that the kernel trick used by SVM alleviates the need to find explicit expression of $\phi(.)$ to compute the transformation

The Kernel Trick

- Recall the SVM optimization problem

$$\max_{\alpha} \quad \mathcal{J}(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i^T \mathbf{x}_j)$$

$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, k$$

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

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Define the kernel function K by

Mercer's Condition

- For which kernels does there exist a pair $\{H;\phi(.)\}$ with the valid geometric properties (e.g., nonnegative dot-product) for a transformation satisfied, and for which does there not?

- *Mercer's Condition for Kernels*
  - There exists a mapping $\phi(.)$ and an expansion

$$K(x,y) = \sum_i \phi_i(x)\phi_i(y)$$

iff for any g(x) such that

$$\int g(x)^2 dx \quad \text{is finite}$$

then

$$\int K(x,y)g(x)g(y)dxdy \geq 0$$

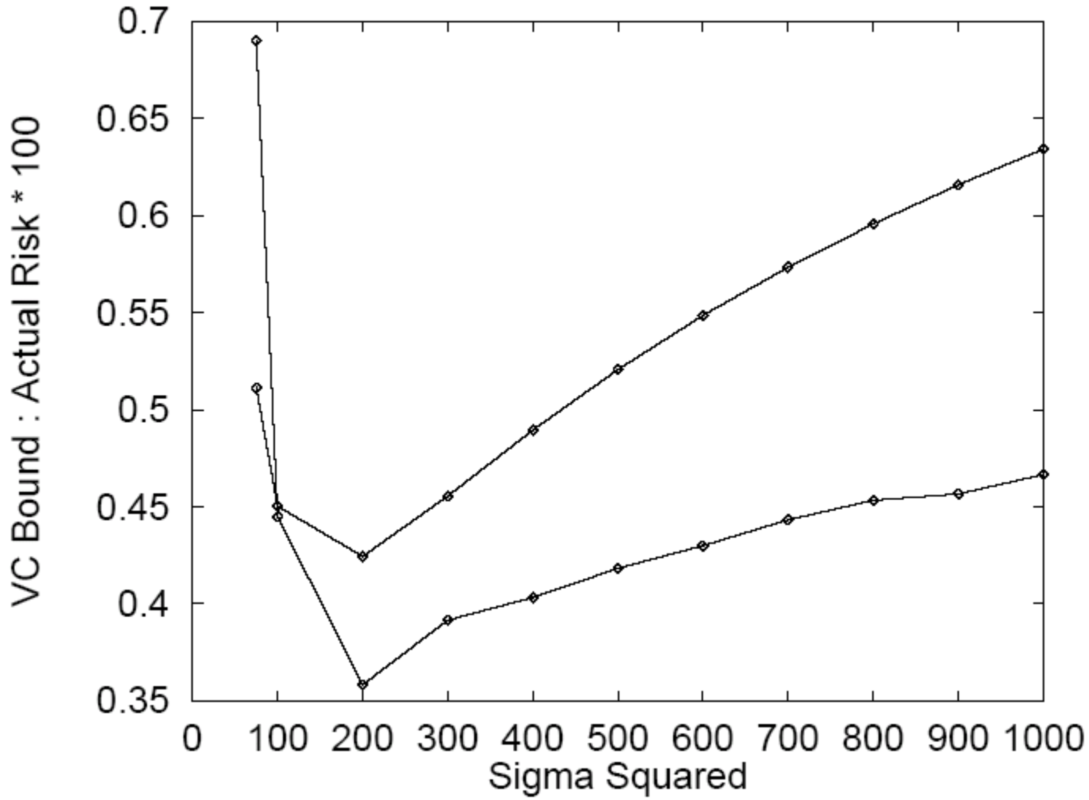
The VC Dimension of SVMs

- We will call any kernel that satisfies Mercer's condition a positive kernel, and the corresponding space *H* the embedding space.

- We will also call any embedding space with minimal dimension for a given kernel a "minimal embedding space".

- Theorem: *Let K be a positive kernel which corresponds to a minimal embedding space H. Then the VC dimension of the corresponding support vector machine (where the error penalty C is allowed to take all values) is* $dim(H) + 1$

VC and the Actual Risk



- It is striking that the two curves have minima in the same place: thus in this case, the VC bound, although loose, seems to be nevertheless predictive.

What You Should Know

- Sample complexity varies with the learning setting
  - Learner actively queries trainer
  - Examples provided at random
- Within the PAC learning setting, we can bound the probability that learner will output hypothesis with given error
  - For ANY consistent learner (case where c in H)
  - For ANY "best fit" hypothesis (agnostic learning, where perhaps c not in H)
- VC dimension as measure of complexity of H
- Quantitative bounds characterizing bias/variance in choice of H
  - but the bounds are quite loose...
- Mistake bounds in learning
- Conference on Learning Theory: http://www.learningtheory.org