Learning Theory

Preview

- "No free lunch" theorems
- Bias and variance
- PAC learning
- VC dimension
- Support vector machines

"No Free Lunch" Theorems

$$Acc_G(L) = \text{Generalization accuracy of learner } L$$
$$= \text{Accuracy of } L \text{ on non-training examples}$$
$\mathcal{F}$ = Set of all possible concepts, $y = f(\mathbf{x})$

Theorem: For any learner L, $\frac{1}{|\mathcal{F}|} \sum_{\mathcal{F}} Acc_G(L) = \frac{1}{2}$
(given any distribution $\mathcal{D}$ over $\mathbf{x}$ and training set size n)

Proof sketch: Given any training set S:
For every concept f where $Acc_G(L) = \frac{1}{2} + \delta$,
there is a concept f' where $Acc_G(L) = \frac{1}{2} - \delta$.
$\forall \mathbf{x} \in S, f'(\mathbf{x}) = f(\mathbf{x}) = y.$ $\quad \forall \mathbf{x} \notin S, f'(\mathbf{x}) = \neg f(\mathbf{x}).$

Corollary: For any two learners L_1, L_2:
If $\exists$ learning problem s.t. $Acc_G(L_1) > Acc_G(L_2)$
Then $\exists$ learning problem s.t. $Acc_G(L_2) > Acc_G(L_1)$

What Does This Mean in Practice?

- Don't expect your favorite learner to always be best
- Try different approaches and compare
- But how could (say) a multilayer perceptron be less accurate than a single-layer one?

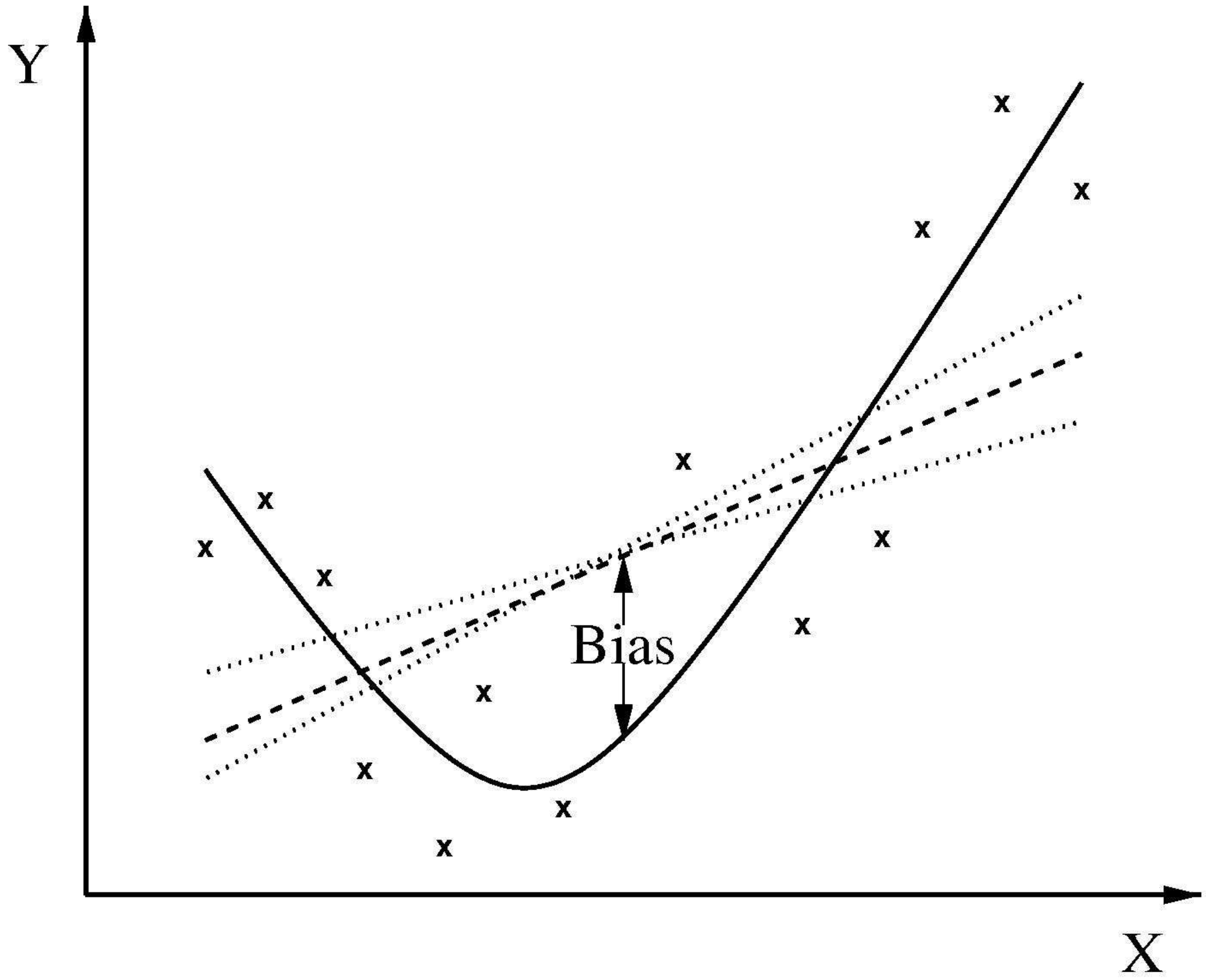
Bias and Variance

- Bias-variance decomposition is key tool for understanding learning algorithms
- Helps explain why simple learners can outperform powerful ones
- Helps explain why model ensembles outperform single models
- Helps understand & avoid overfitting
- Standard decomposition for squared loss
- Can be generalized to zero-one loss

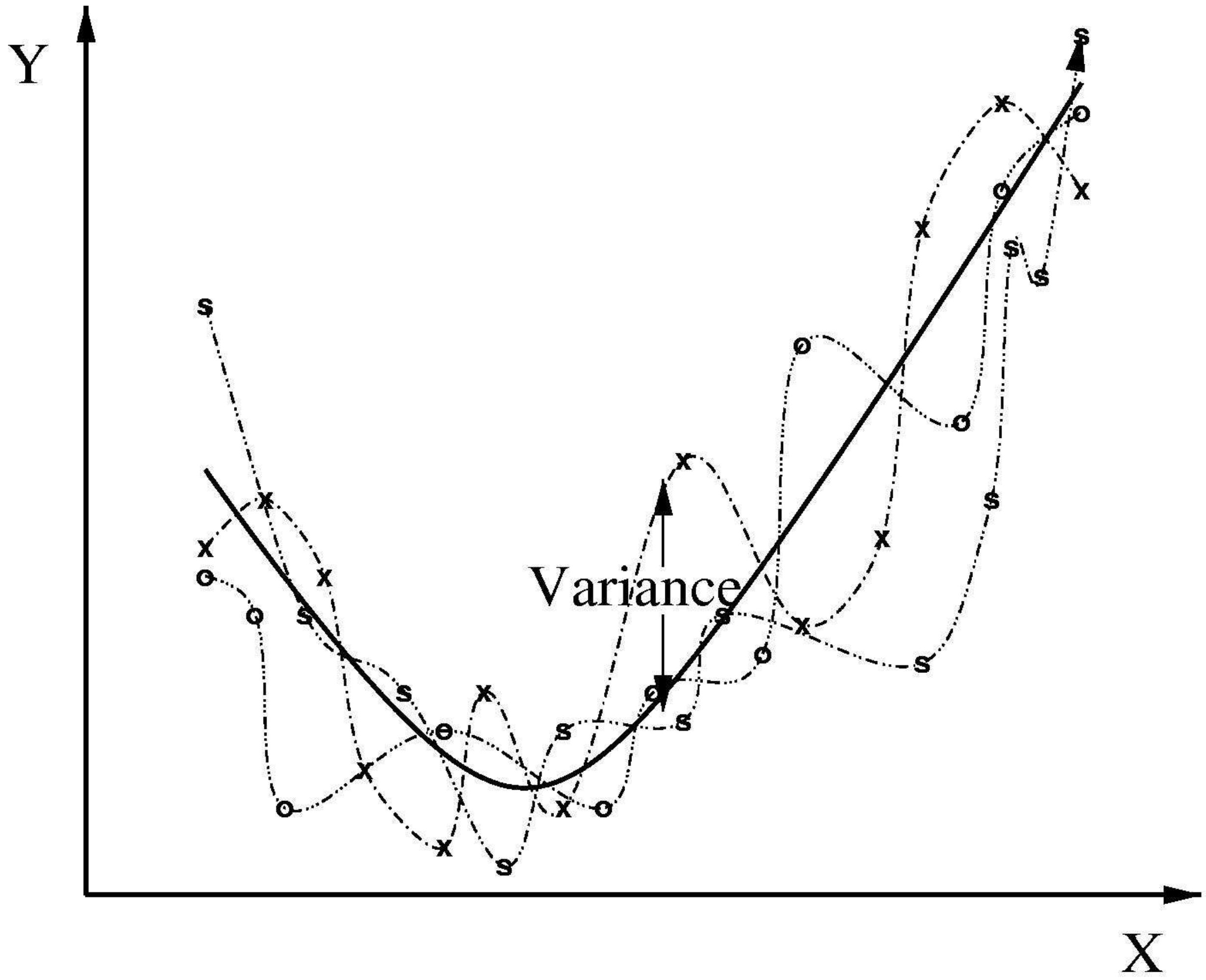
Definitions

- Given training set: $\{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$
- Learner induces model: $y = f(\mathbf{x})$
- Loss measures quality of learner's predictions
  - Squared loss: $L(t, y) = (t - y)^2$
  - Absolute loss: $L(t, y) = |t - y|$
  - Zero-one loss: $L(t, y) = 0$ if $y = t$, 1 otherwise
  - Etc.
- Loss = Bias + Variance + Noise
  (This lecture: ignore noise; see paper)

Bias



Variance



Decomposition for squared loss

$$
\begin{aligned}
(t-y)^2 &= (t-\overline{y}+\overline{y}-y)^2 \\
&= (t-\overline{y})^2 + (\overline{y}-y)^2 + 2(t-\overline{y})(\overline{y}-y)
\end{aligned}
$$

$$
\begin{aligned}
E[(t-y)^2] &= (t-\overline{y})^2 + E[(\overline{y}-y)^2] \\
\text{Exp. loss} &= \text{Bias} \qquad + \text{Variance}
\end{aligned}
$$

(Expectations are over training sets)

How to generalize this to other loss funcs?

$$E[(t-y)^2] = (t-\overline{y})^2 + E[(\overline{y}-y)^2]$$

$$\begin{array}{rcll} (a-b)^2 & \rightarrow & L(a,b) & \\ E[(t-y)^2] & \rightarrow & E[L(t,y)] & \text{(Exp. loss)} \\ (t-\overline{y})^2 & \rightarrow & L(t,\overline{y}) & \text{(Bias)} \\ E[(\overline{y}-y)^2] & \rightarrow & E[L(\overline{y},y)] & \text{(Variance)} \end{array}$$

But what should $\overline{y}$ be?

Define **Main Prediction**:
Prediction with min average loss relative to all predictions

$$\overline{y}_L = \operatorname*{argmin}_{y'} E[L(y, y')]$$

- Squared loss: $\overline{y}$ = Mean
- Absolute loss: $\overline{y}$ = Median
- Zero-one loss: $\overline{y}$ = Mode

Generalized definitions

Bias = Loss incurred by main prediction = $L(t, \overline{y})$

Variance = Average loss incurred by prediction relative to main prediction = $E[L(\overline{y}, y)]$

These definitions have all the required properties.

For zero-one loss:

$$\textbf{Bias} = \begin{cases} 0 \text{ if main prediction is correct} \\ 1 \text{ otherwise} \end{cases}$$

Variance = Prob(Prediction $\neq$ Main pred) = $P(y \neq \overline{y})$

Can we decompose zero-one loss into these?

Assume two-class problem.

Bias = 0 $\Rightarrow$ **Loss = Bias + Variance**

Loss $= P(y \neq t)$ Variance $= P(y \neq \overline{y})$

Bias $= 0 \Leftrightarrow \overline{y} = \mathrm{t}$

Bias = 1 $\Rightarrow$ **Loss = Bias − Variance**

Loss $= P(y \neq t) = 1 - P(y = t) = 1 - P(y \neq \overline{y})$

because if $\overline{y} \neq t$ then $y = t \Leftrightarrow y \neq \overline{y}$.

Increasing variance can reduce loss!

Can we generalize this further?

$$\text{Loss} = \text{Bias} + c\ \text{Variance}$$

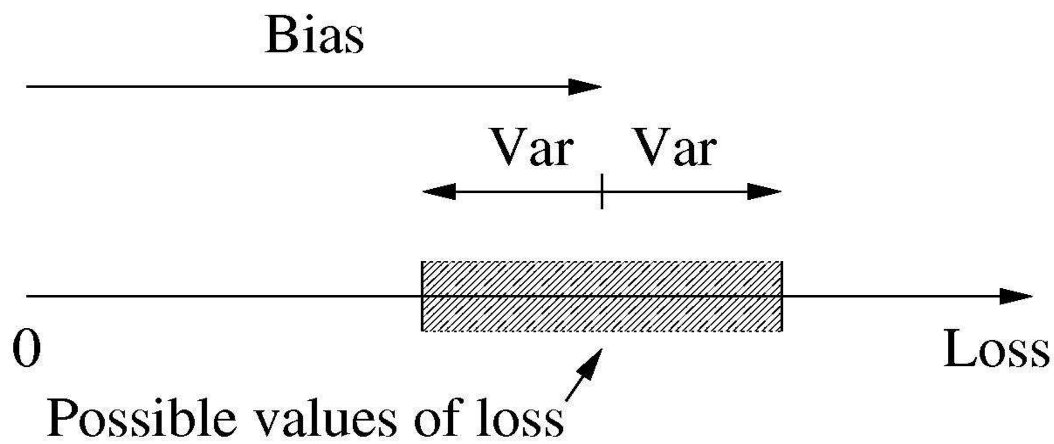
where c = 1 if Bias = 0, otherwise see below

- **Applies to:**
  - Squared loss: $c = 1$
  - Two-class problems: $c = -1$
  - Multiclass problems: $c = -P(y = t | y \neq \overline{y})$
  - Variable costs: $c = -L(t, \overline{y})/L(\overline{y}, t)$

Metric loss functions

- What about loss functions where decomposition does not apply?
- For any metric loss function:

$$\text{Loss} \leq \text{Bias} + \text{Variance}$$
$$\text{Loss} \geq \text{Max}\,\{\text{Bias} - \text{Var},\ \text{Var} - \text{Bias}\}$$



PAC Learning

- Overfitting happens because training error is bad estimate of generalization error

→ Can we infer something about generalization error from training error?

- Overfitting happens when the learner doesn't see "enough" examples

→ Can we estimate how many examples are enough?

Problem Setting

Given:

- Set of instances X
- Set of hypotheses H
- Set of possible target concepts C
- Training instances generated by a fixed, unknown probability distribution $\mathcal{D}$ over X

Learner observes sequence D of training examples $\langle x, c(x) \rangle$, for some target concept $c \in C$

- Instances x are drawn from distribution $\mathcal{D}$
- Teacher provides target value $c(x)$ for each

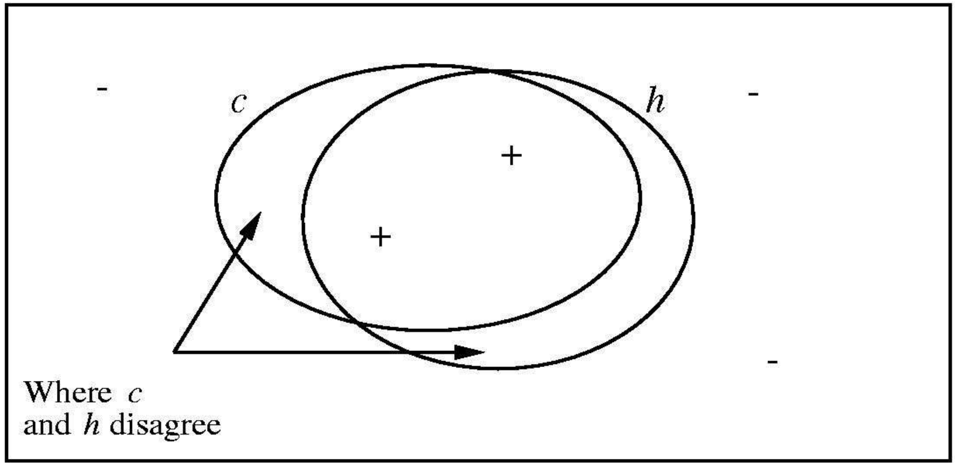
Learner must output a hypothesis h estimating c

- h is evaluated by its performance on subsequent instances drawn according to $\mathcal{D}$

Note: probabilistic instances, noise-free classifications

True Error of a Hypothesis

Instance space X



Definition: The **true error** (denoted $error_{\mathcal{D}}(h)$) of hypothesis h with respect to target concept c and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

Two Notions of Error

Training error of hypothesis h with respect to target concept c

- How often $h(x) \neq c(x)$ over training instances

True error of hypothesis h with respect to c

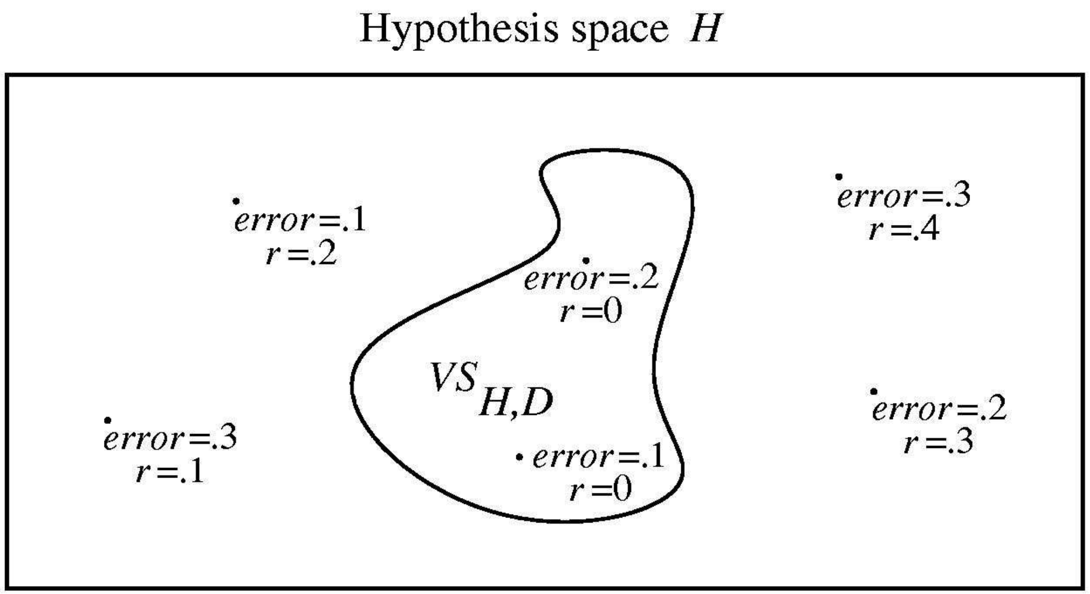
- How often $h(x) \neq c(x)$ over future random instances

Our concern:

- Can we bound the true error of h given the training error of h?
- First consider when training error of h is zero

Version Spaces

Version Space $VS_{H,D}$**:**
Subset of hypotheses in H consistent with training data D



(r = training error, $error$ = true error)

How Many Examples Are Enough?

Theorem:
If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples of some target concept c, then for any $0 \leq \epsilon \leq 1$, the probability that $VS_{H,D}$ contains a hypothesis with error greater than ϵ is less than

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

Proof sketch:
Prob(1 hyp. w/ error $> \epsilon$ consistent w/ 1 ex.) $< 1 - \epsilon \leq e^{-\epsilon}$
Prob(1 hyp. w/ error $> \epsilon$ consistent with m exs.) $< e^{-\epsilon m}$
Prob(1 of $|H|$ hyps. consistent with m exs.) $< |H|e^{-\epsilon m}$

Interesting! This bounds the probability that any consistent learner will output a hypothesis h with $error(h) \geq \epsilon$

If we want this probability to be at most δ

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

then

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

Learning Conjunctions

How many examples are sufficient to ensure with probability at least $(1-\delta)$ that every h in $VS_{H,D}$ satisfies $error_{\mathcal{D}}(h) \leq \epsilon$?

Use our theorem:

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

Suppose H contains conjunctions of constraints on up to n Boolean attributes (i.e., n literals). Then $|H| = 3^n$, and

$$\begin{aligned} m &\geq \frac{1}{\epsilon}(\ln 3^n + \ln(1/\delta)) \\ &\geq \frac{1}{\epsilon}(n \ln 3 + \ln(1/\delta)) \end{aligned}$$

How About *PlayTennis*?

1 attribute with 3 values (outlook)
9 attributes with 2 values (temp, humidity, wind, etc.)
Language: Conjunction of features or null concept

$$|H| = 4 \times 3^9 + 1 = 78733$$

$$m \geq \frac{1}{\epsilon}(\ln 78733 + \ln(1/\delta))$$

If we want to ensure that with probability 95%,
VS contains only hypotheses with $error_{\mathcal{D}}(h) \leq 10\%$,
then it is sufficient to have m examples, where

$$m \geq \frac{1}{0.1}(\ln 78733 + \ln(1/.05)) = 143$$

(# examples in domain: $3 \times 2^9 = 1536$)

PAC Learning

Consider a class C of possible target concepts defined over a set of instances X of length n, and a learner L using hypothesis space H.

Definition: C is **PAC-learnable** by L using H iff 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 $size(c)$.

Agnostic Learning

So far, assumed $c \in H$

Agnostic learning setting: don't assume $c \in H$

- What can we say in this case?
  - Hoeffding bounds:

    $$Pr[error_{\mathcal{D}}(h) > error_D(h) + \epsilon] \leq e^{-2m\epsilon^2}$$
  - For hypothesis space H:

    $$Pr[error_{\mathcal{D}}(h_{best}) > error_D(h_{best}) + \epsilon] \leq |H|e^{-2m\epsilon^2}$$
- What is the sample complexity in this case?

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

VC Dimension

- What about hypotheses with numeric parameters?
- Solution: Use VC dimension instead of $\ln |H|$

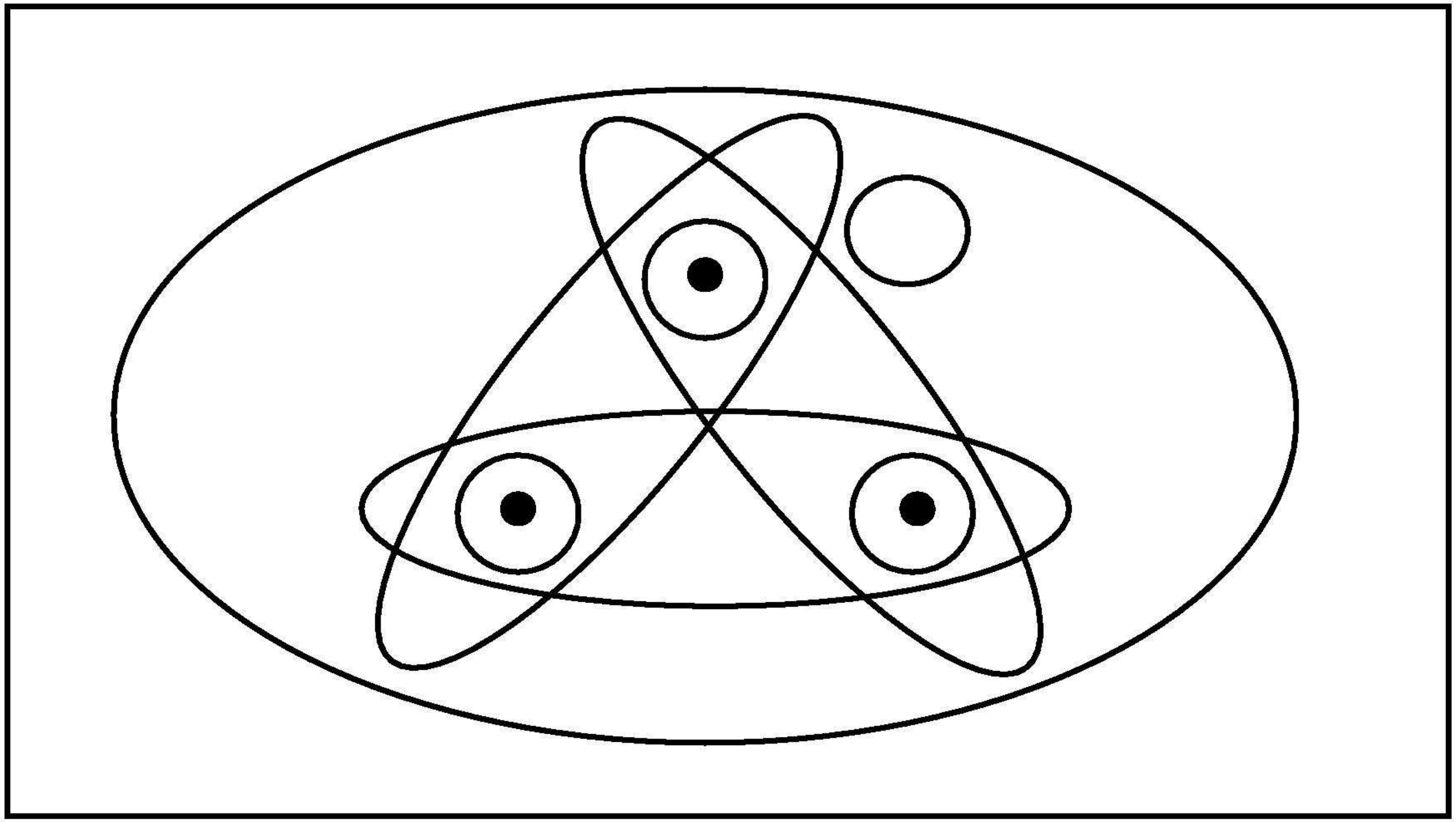
Shattering a Set of Instances

Definition: a **dichotomy** of a set S is a partition of S into two disjoint subsets.

Definition: a set of instances S is **shattered** by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.

Three Instances Shattered

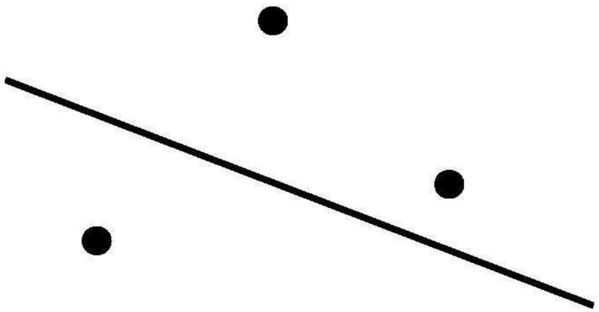
Instance space X



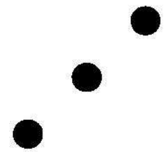
The Vapnik-Chervonenkis Dimension

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 Dim. of Linear Decision Surfaces



(a)



(b)

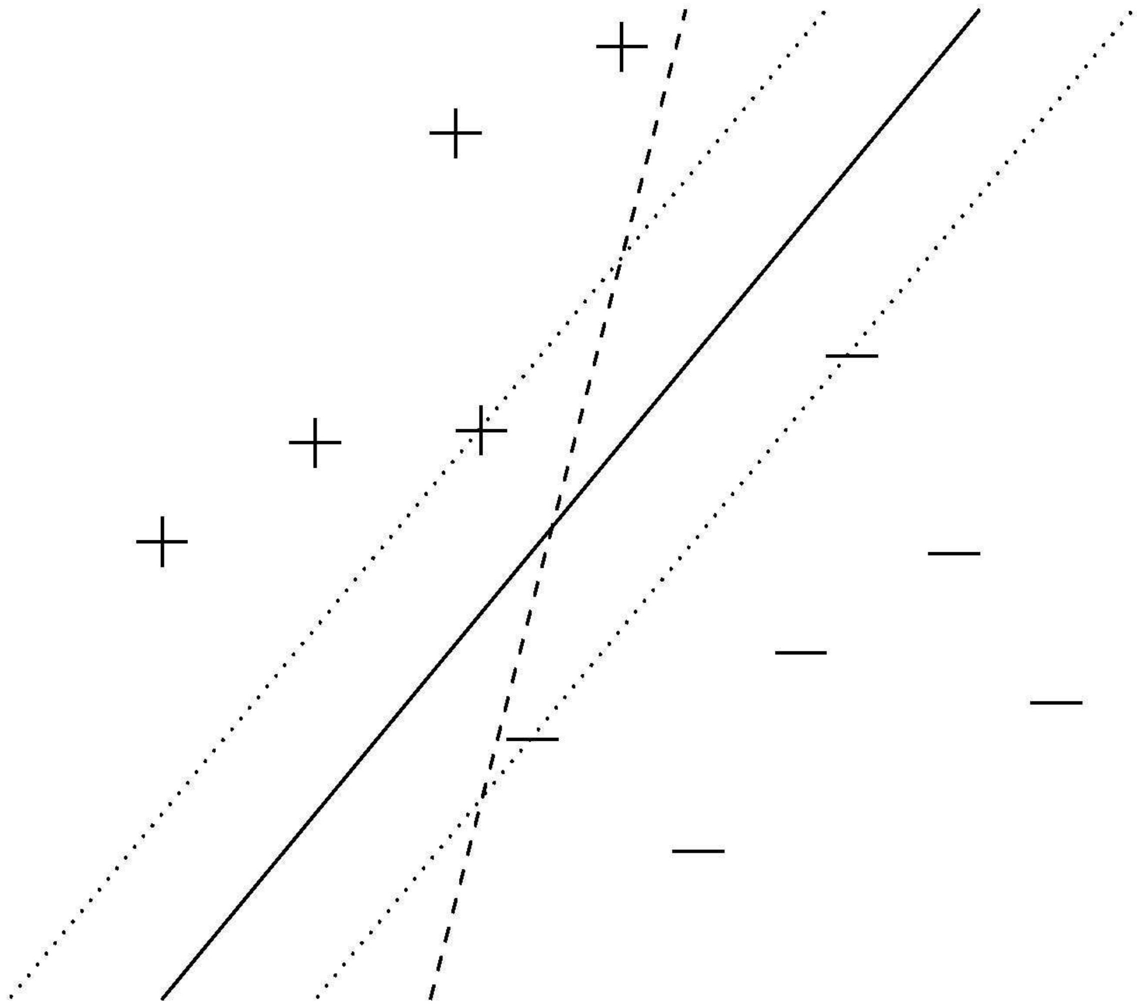
VC dim. of hyperplane in d-dimensional space is $d+1$

Sample Complexity from VC Dimension

How many randomly drawn examples suffice to guarantee error of at most ϵ with probability at least $(1 - \delta)$?

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

Support Vector Machines



Support Vector Machines

- Many different hyperplanes can separate positive and negative examples
- Choose hyperplane with maximum margin
- **Margin**: Min. distance between plane and example
- Bound on VC dimension decreases with margin
- **Support vectors:** Examples that determine the plane
- $E[error_{\mathcal{D}}(h)] \leq \frac{E[\#support\ vectors]}{\#training\ vectors - 1}$
- Noisy data: use slack variables
- Avoids overfitting even in very high-dimensional spaces (e.g., text)
- Non-linear: augment data with derived features

Learning Theory: Summary

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- Bias and variance
- PAC learning
- VC dimension
- Support vector machines