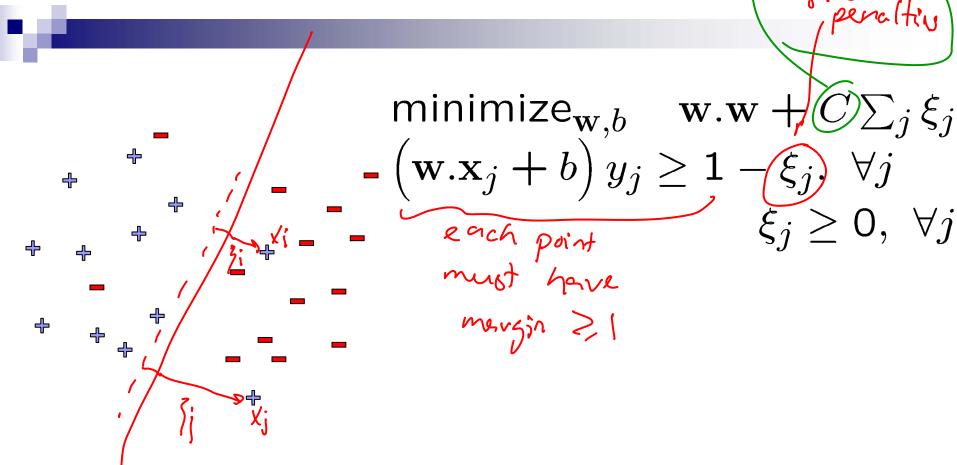
SVMs, Duality and the Kernel Trick (cont.)

Machine Learning – 10701/15781
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February 28th, 2007

SVMs reminder





Dual SVM formulation – the non-separable case

one di Ru Rach data Point

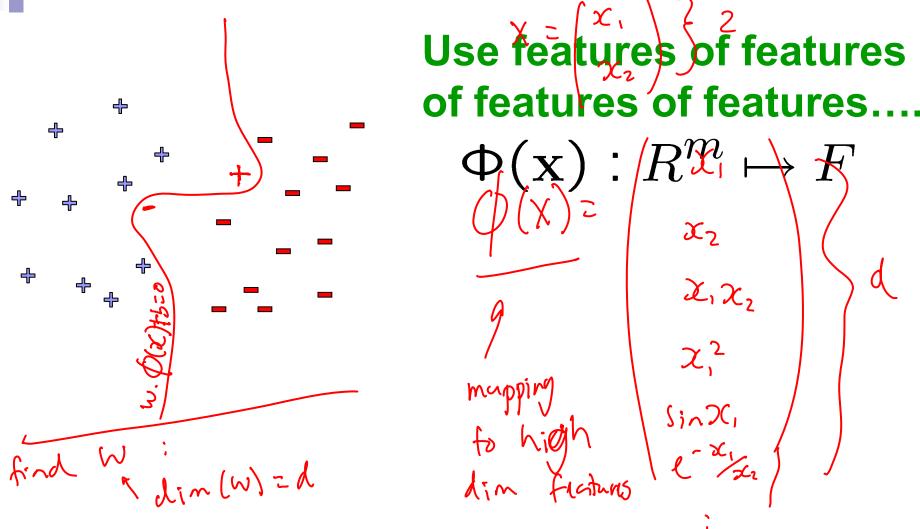
separable case: only different

 $\mathbf{w} = \sum_{i} \alpha_i y_i \mathbf{x}_i$ $b = y_k - \mathbf{w}.\mathbf{x}_k$ for any k where $C > \alpha_k > 0$

intuitively, don't give ave too large

alphas that

Reminder from last time: What if the data is not linearly separable?



Feature space can get really large really quickly!

Dual formulation only depends on dot-products, not on w!

$$\max_{\alpha} \max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i} x_{j}$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C \geq \alpha_{i} \geq 0$$

$$\phi(x_{i}) \cdot \phi(x_{j}) = K(x_{i}, x_{j})$$

$$\max_{\alpha} \max_{\beta} \max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} K(x_{i}, x_{j})$$

$$K(x_{i}, x_{j}) = \phi(x_{i}) \cdot \phi(x_{j})$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C \geq \alpha_{i} \geq 0$$

$$C \geq \alpha_{i} \geq 0$$

Dot-product of polynomials

$$\mathcal{N} = \begin{pmatrix} u_1 \\ h_2 \end{pmatrix}$$

$$V = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$

 $\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree d}$

$$\frac{d^{2}}{d^{2}} = \frac{d(u)^{2}}{d(u)^{2}} = \frac{d(u)^{2$$

degree =d
$$K(\mu, \nu) = \phi(\mu) \cdot \phi(\nu) = (\mu, \nu)^d$$

= $O(d)$ multiplications

Finally: the "kernel trick"!

maximize_{$$\alpha$$} $\sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$

$$K(\mathbf{x}_{i}, \mathbf{x}_{j}) = \Phi(\mathbf{x}_{i}) \cdot \Phi(\mathbf{x}_{j})$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C \ge \alpha_i \ge 0$$

- Never represent features explicitly
 - Compute dot products in closed form



Constant-time high-dimensional dotproducts for many classes of features

$$\mathbf{w} = \sum_{i} \alpha_{i} y_{i} \Phi(\mathbf{x}_{i})$$

$$b = y_k - \mathbf{w}.\Phi(\mathbf{x}_k)$$

for any k where $C > \alpha_k > 0$

- Very interesting theory Reproducing Kernel Hilbert Spaces
 - □ Not covered in detail in 10701/15781, more in 10702

Common kernels



Polynomials of degree d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d / \!\!/$$

Polynomials of degree up to d
$$K(\mathbf{u},\mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^d$$

Gaussian kernels

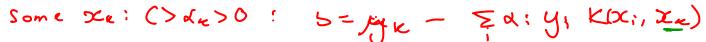
Gaussian Kernels
$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_{2}^{2}}{2\sigma^{2}}\right)$$

Sigmoid

$$K(\mathbf{u}, \mathbf{v}) = \tanh(\eta \mathbf{u} \cdot \mathbf{v} + \nu)$$

Overfitting?

- ra.
 - Huge feature space with kernels, what about overfitting???
 - Maximizing margin leads to sparse set of support vectors
 - Some interesting theory says that SVMs search for simple hypothesis with large margin
 - Often robust to overfitting



What about at classification time

The Proof of the Proof of the we are in trouble!

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- Recall classifier: sign(w.Φ(x)+b)
- Using kernels we are cool!

$$K(\mathbf{u}, \mathbf{v}) = \Phi(\mathbf{u}) \cdot \Phi(\mathbf{v})$$

$$w.\phi(\mathbf{x}) + b = (7 \text{ diy: } \Phi(\mathbf{x}i)) \cdot \Phi(\mathbf{x}) + 5$$

$$= 7 \text{ diy: } \Phi(\mathbf{x}i) \cdot \Phi(\mathbf{x}) + 5$$

$$= 7 \text{ diy: } \Phi(\mathbf{x}i) \cdot \Phi(\mathbf{x}) + 5$$

$$\mathbf{w} = \sum_{i} \alpha_{i} y_{i} \Phi(\mathbf{x}_{i})$$
 $b = y_{k} - \mathbf{w}.\Phi(\mathbf{x}_{k})$
for any k where $C > \alpha_{k} > 0$

= Z X; M; K(X, X;) +6 >

SVMs with kernels

- input
 - Choose a set of features and kernel function
 - lacksquare Solve dual problem to obtain support vectors $lpha_{i}$
 - At classification time, compute:

$$\mathbf{w} \cdot \Phi(\mathbf{x}) = \sum_i \alpha_i y_i K(\mathbf{x}, \mathbf{x}_i)$$

$$b = y_k - \sum_i \alpha_i y_i K(\mathbf{x}_k, \mathbf{x}_i)$$
 for any k where $C > \alpha_k > 0$

Remember kernel regression

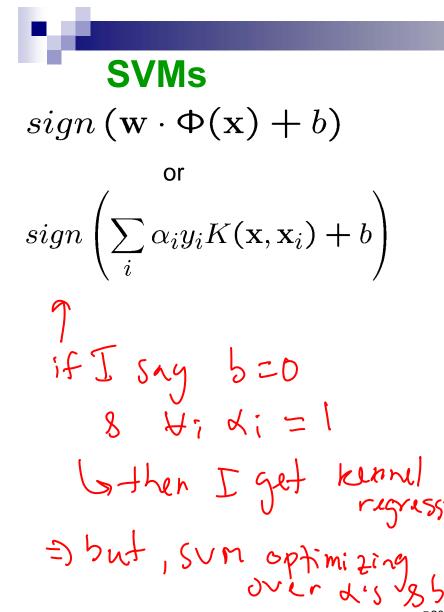


Remember kernel regression???

- 1. $W_i = \exp(-D(x_i, query)^2 / K_w^2)$
- 2. How to fit with the local points?

Predict the weighted average of the outputs: predict = $\sum w_i y_i / \sum w_i$

SVMs v. Kernel Regression



Kernel Regression

$$sign\left(\frac{\sum_{i} y_{i} K(\mathbf{x}, \mathbf{x}_{i})}{\sum_{j} K(\mathbf{x}, \mathbf{x}_{j})}\right)$$

$$\frac{1}{Z_{i}} k(x_{i} x_{i}) = x(x)$$



SVMs v. Kernel Regression



SVMs

$$sign\left(\mathbf{w}\cdot\Phi(\mathbf{x})+b\right)$$
 or

Kernel Regression

$$sign\left(\frac{\sum_{i} y_{i} K(\mathbf{x}, \mathbf{x}_{i})}{\sum_{i} K(\mathbf{x}, \mathbf{x}_{i})}\right)$$

Differences:

- SVMs:
 - \square Learn weights α_i (and bandwidth)
 - □ Often sparse solution

KR:

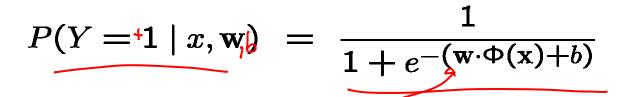
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- ☐ Fixed "weights", learn bandwidth
- Solution may not be sparse
- Much simpler to implement

What's the difference between SVMs and Logistic Regression?

	SVMs	Logistic Regression
Loss function		
High dimensional features with kernels		actually yes

Kernels in logistic regression



$$\mathbf{w} = \sum_{i} \alpha_{i} \Phi(\mathbf{x}_{i})$$
 Define weights in terms of support vectors:
$$\mathbf{w} = \sum_{i} \alpha_{i} \Phi(\mathbf{x}_{i})$$

$$P(Y = 1 \mid x, \mathbf{w}) = \frac{1}{1 + e^{-(\sum_{i} \alpha_{i} \Phi(\mathbf{x}_{i}) \cdot \Phi(\mathbf{x}) + b)}}$$

$$\chi(\chi, \chi_{i}) = \emptyset(\chi_{i}) \cdot \emptyset(\chi) = \frac{1}{1 + e^{-(\sum_{i} \alpha_{i} K(\mathbf{x}, \mathbf{x}_{i}) + b)}}$$

$$\text{Derive simple gradient descent rule on } \alpha_{i} \alpha_$$

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What's the difference between SVMs and Logistic Regression? (Revisited)

	SVMs	Logistic Regression
Loss function	Hinge loss after	Log-loss neverzend
High dimensional features with kernels	Yes!!	Yes!
many disco		

What you need to know

- NA.
 - Dual SVM formulation
 - □ How it's derived (intuition)
 - The kernel trick
 - Derive polynomial kernel
 - Common kernels
 - Kernelized logistic regression
 - Differences between SVMs and logistic regression
 - D SVMS with kernels v. Kernel regression

Announcements



Class projects out next week

Learning Theory

PAC-learning, VC Dimension and Margin-based Bounds

Machine Learning – 10701/15781
Carlos Guestrin
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What now...



- We have explored many ways of learning from data
- But...
 - ☐ How good is our classifier, really?
 - □ How much data do I need to make it "good enough"?

A simple setting...

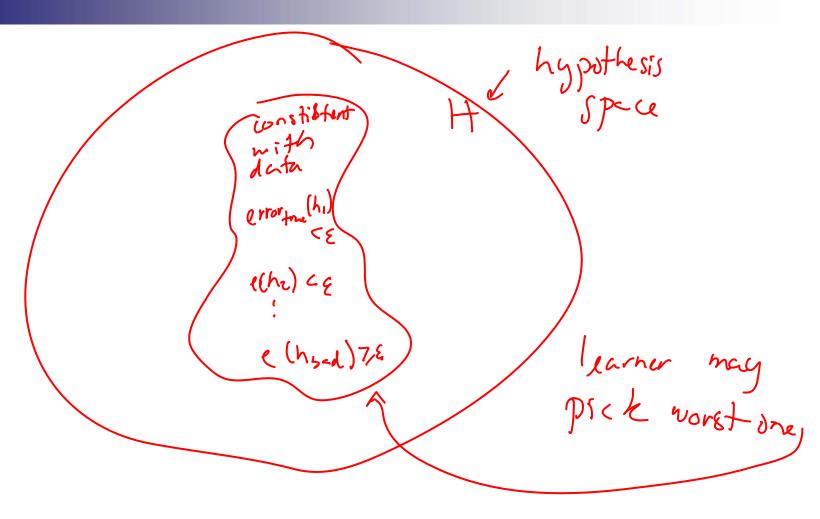


- Classification
 - □ m data points
 - of depth d) on categoricals data
- A learner finds a hypothesis h that is consistent with training data
 - Gets zero error in training error_{train}(h) = 0
- What is the probability that h has more than ε true error?
 - □ error_{true}(h) γε

How likely is a bad hypothesis to get *m* data points right?

- Hypothesis h that is consistent with training data got m i.i.d. points right
- Prob. h with $error_{true}(h) \ge \epsilon$ gets one data point right $P(h \text{ gets 1 point right}) \le 1-\epsilon$
- Prob. h with error_{true}(h) ξ ϵ gets m data points right $P(h \text{ gets } m \text{ i.i.d. points right}) \leq (1-\xi)^m$

But there are many possible hypothesis that are consistent with training data

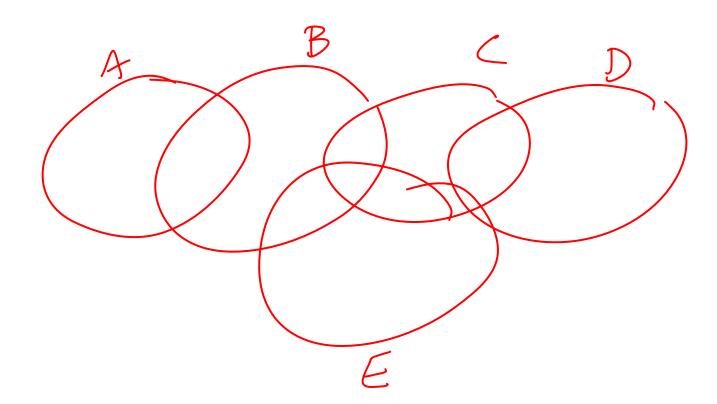


How likely is learner to pick a bad hypothesis

- Prob. h with error_{true}(h) $\gtrsim \epsilon$ gets m data points right $P(badh gts m points right) <math>\leq (1-\epsilon)^m$
- There are k hypothesis consistent with data = (h, -- 4,)
 - □ How likely is learner to pick a bad one?

Union bound

■ P(A or B or C or D or ...) $\leq P(A) + P(B) + P(C) + \cdots$



How likely is learner to pick a bad hypothesis

- Prob. h; with $error_{true}(h) \ge \epsilon$ gets m data points right $P(\ell_{+}(h)) = 8$ consistent with m data points $P(\ell_{+}(h)) = 8$ consistent with m data points $P(\ell_{+}(h)) = 8$
- There are *k* hypothesis consistent with data
 - □ How likely is learner to pick a bad one?

P(Pt(N)) & 8 hiconsident
$$V$$
 Pt (n)) & 8 consistent V -... V P(hk) > 8 8 consistent)

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Review: Generalization error in finite hypothesis spaces [Haussler '88]

Theorem: Hypothesis space H finite, dataset D with m i.i.d. samples, $0 < \varepsilon < 1$: for any learned hypothesis h that is consistent on the training data:

$$P(\text{error}_{true}(h) \ge \epsilon) \le |H|e^{-m\epsilon}$$

m -s incresses =) Prob. make a Sad de Cision de cresse 2.2 exponentially East 11+1 -> incresses 45

=) Chances of making a bad decision increase linearly with 141

Using a PAC bound guarantee with high prob. PAC: probably Approximately Corned [vant: erro-free (h) \in \in \in \in \text{ grantee with prob.}] - J

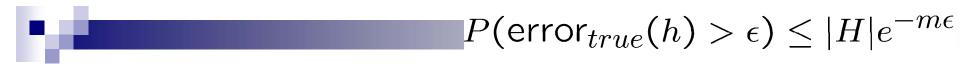
- Typically, 2 use cases: $P(error_{true}(h) > \epsilon) \le |H|e^{-m\epsilon}$
 - □ 1: Pick ε and δ, give you \underline{m}
 - $_{1}$ \square 2: Pick m and δ , give you ϵ

Review: Generalization error in finite hypothesis spaces [Haussler '88]

■ **Theorem**: Hypothesis space H finite, dataset D with m i.i.d. samples, $0 < \varepsilon < 1$: for any learned hypothesis h that is consistent on the training data:

$$P(\text{error}_{true}(h) > \epsilon) \le |H|e^{-m\epsilon}$$

Limitations of Haussler '88 bound



Consistent classifier

Size of hypothesis space

What if our classifier does not have zero error on the training data?

- A learner with zero training errors may make mistakes in test set
- What about a learner with *error*_{train}(h) in training set?

Simpler question: What's the expected error of a hypothesis?

The error of a hypothesis is like estimating the parameter of a coin!

■ Chernoff bound: for m i.i.d. coin flips, $x_1,...,x_m$, where x_i 2 {0,1}. For 0< ϵ <1:

$$P\left(\theta - \frac{1}{m}\sum_{i} x_{i} > \epsilon\right) \leq e^{-2m\epsilon^{2}}$$

Using Chernoff bound to estimate error of a single hypothesis

$$\left| P\left(\theta - \frac{1}{m} \sum_{i} x_i > \epsilon\right) \le e^{-2m\epsilon^2} \right|$$

But we are comparing many hypothesis: **Union bound**

For each hypothesis h_i:

$$P\left(\text{error}_{true}(h_i) - \text{error}_{train}(h_i) > \epsilon\right) \le e^{-2m\epsilon^2}$$

What if I am comparing two hypothesis, h₁ and h₂?

Generalization bound for |H| hypothesis

Theorem: Hypothesis space H finite, dataset D with m i.i.d. samples, 0 < ε < 1 : for any learned hypothesis h:</p>

$$P\left(\operatorname{error}_{true}(h) - \operatorname{error}_{train}(h) > \epsilon\right) \le |H|e^{-2m\epsilon^2}$$

PAC bound and Bias-Variance tradeoff

$$P\left(\operatorname{error}_{true}(h) - \operatorname{error}_{train}(h) > \epsilon\right) \le |H|e^{-2m\epsilon^2}$$

or, after moving some terms around,

with probability at least 1-
$$\delta$$
:
$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2m}}$$

Important: PAC bound holds for all h, but doesn't guarantee that algorithm finds best h!!!

What about the size of the hypothesis space?

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

How large is the hypothesis space?

Boolean formulas with *n* binary features



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

Number of decision trees of depth k



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

Recursive solution

```
Given n attributes

H_k = \text{Number of decision trees of depth k}

H_0 = 2

H_{k+1} = (\text{\#choices of root attribute})^*

(\text{\# possible left subtrees})^*

(\text{\# possible right subtrees})

= n^* H_k^* H_k

Write L_k = \log_2 H_k

L_0 = 1

L_{k+1} = \log_2 n + 2L_k

So L_k = (2^k-1)(1+\log_2 n) + 1
```

PAC bound for decision trees of depth k

$$m \ge \frac{\ln 2}{2\epsilon^2} \left((2^k - 1)(1 + \log_2 n) + 1 + \ln \frac{1}{\delta} \right)$$

- Bad!!!
 - □ Number of points is exponential in depth!

■ But, for *m* data points, decision tree can't get too big...

Number of leaves never more than number data points

Number of decision trees with k leaves



H_k = Number of decision trees with k leaves

$$H_0 = 2$$

$$H_{k+1} = n \sum_{i=1}^{k} H_i H_{k+1-i}$$

Loose bound:

$$H_k = n^{k-1}(k+1)^{2k-1}$$

Reminder:

|DTs depth
$$k| = 2 * (2n)^{2^k-1}$$

PAC bound for decision trees with k leaves – Bias-Variance revisited

$$H_k = n^{k-1}(k+1)^{2k-1}$$
 $\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln \frac{1}{\delta}}{2m}}$

$$\mathsf{error}_{true}(h) \leq \mathsf{error}_{train}(h) + \sqrt{rac{(k-1) \ln n + (2k-1) \ln (k+1) + \ln rac{1}{\delta}}{2m}}$$

What did we learn from decision trees?



Bias-Variance tradeoff formalized

$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{(k-1)\ln n + (2k-1)\ln(k+1) + \ln\frac{1}{\delta}}{2m}}$$

Moral of the story:

Complexity of learning not measured in terms of size hypothesis space, but in maximum *number of points* that allows consistent classification

- \square Complexity m no bias, lots of variance
- □ Lower than m some bias, less variance

What about continuous hypothesis spaces?

$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{\ln|H| + \ln\frac{1}{\delta}}{2m}}$$

- Continuous hypothesis space:
 - $\square |H| = 1$
 - □ Infinite variance???
- As with decision trees, only care about the maximum number of points that can be classified exactly!

How many points can a linear boundary classify exactly? (1-D)

How many points can a linear boundary classify exactly? (2-D)

How many points can a linear boundary classify exactly? (d-D)

PAC bound using VC dimension



- Number of training points that can be classified exactly is VC dimension!!!
 - Measures relevant size of hypothesis space, as with decision trees with k leaves

$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{VC(H)\left(\ln\frac{2m}{VC(H)} + 1\right) + \ln\frac{4}{\delta}}{m}}$$

Shattering a set of points



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.

VC 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 $VC(H) \equiv \infty$.

Examples of VC dimension



- Linear classifiers:
 - \square VC(H) = d+1, for *d* features plus constant term *b*
- Neural networks
 - □ VC(H) = #parameters
 - Local minima means NNs will probably not find best parameters
- 1-Nearest neighbor?

PAC bound for SVMs



- SVMs use a linear classifier
 - □ For *d* features, VC(H) = d+1:

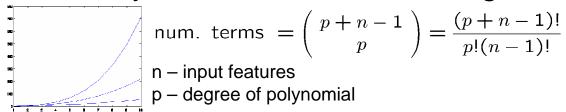
$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{(d+1)\left(\ln\frac{2m}{d+1}+1\right) + \ln\frac{4}{\delta}}{m}}$$

VC dimension and SVMs: Problems!!!

Doesn't take margin into account

$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{(d+1)\left(\ln\frac{2m}{d+1}+1\right) + \ln\frac{4}{\delta}}{m}}$$

- What about kernels?
 - □ Polynomials: num. features grows really fast = Bad bound



□ Gaussian kernels can classify any set of points exactly

Margin-based VC dimension

- H: Class of linear classifiers: w.⊕(x) (b=0)
 - \square Canonical form: min_i |**w**. Φ (**x**_i)| = 1
- $VC(H) = R^2$ w.w
 - □ Doesn't depend on number of features!!!
 - \square R² = max_i $\Phi(\mathbf{x}_i)$. $\Phi(\mathbf{x}_i)$ magnitude of data
 - □ R² is bounded even for Gaussian kernels! bounded VC dimension
- Large margin, low w.w, low VC dimension Very cool!

Applying margin VC to SVMs?

$$\operatorname{error}_{true}(h) \leq \operatorname{error}_{train}(h) + \sqrt{\frac{VC(H)\left(\ln\frac{2m}{VC(H)} + 1\right) + \ln\frac{4}{\delta}}{m}}$$

- $VC(H) = R^2 \mathbf{w.w}$
 - \square R² = max_i $\Phi(\mathbf{x}_i)$. $\Phi(\mathbf{x}_i)$ magnitude of data, doesn't depend on choice of **w**
- SVMs minimize w.w
- SVMs minimize VC dimension to get best bound?
- Not quite right: ⊗
 - Bound assumes VC dimension chosen before looking at data
 - Would require union bound over infinite number of possible VC dimensions...
 - □ But, it can be fixed!

Structural risk minimization theorem

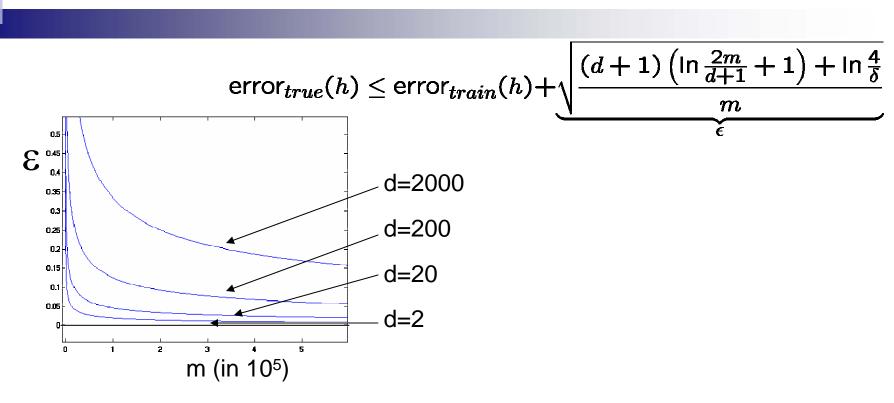


$$\operatorname{error}_{true}^{\gamma}(h) \leq \operatorname{error}_{train}^{\gamma}(h) + C\sqrt{\frac{\frac{R^2}{\gamma^2} \ln m + \ln \frac{1}{\delta}}{m}}$$

 $\operatorname{error}_{train}^{\gamma}(h) = \operatorname{num.}$ points with margin $< \gamma$

- For a family of hyperplanes with margin γ >0
 - w.w 1
- SVMs maximize margin γ + hinge loss
 - Optimize tradeoff training error (bias) versus margin γ (variance)

Reality check – Bounds are loose



- Bound can be very loose, why should you care?
 - ☐ There are tighter, albeit more complicated, bounds
 - □ Bounds gives us formal guarantees that empirical studies can't provide
 - Bounds give us intuition about complexity of problems and convergence rate of algorithms

What you need to know

- MA
 - Finite hypothesis space
 - Derive results
 - Counting number of hypothesis
 - Mistakes on Training data
 - Complexity of the classifier depends on number of points that can be classified exactly
 - □ Finite case decision trees
 - □ Infinite case VC dimension
 - Bias-Variance tradeoff in learning theory
 - Margin-based bound for SVM
 - Remember: will your algorithm find best classifier?