RWTHAACHEN UNIVERSITY

Machine Learning - Lecture 7

Statistical Learning Theory

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Many slides adapted from B. Schiel

Course Outline Fundamentals (2 weeks) Bayes Decision Theory Probability Density Estimation Discriminative Approaches (5 weeks) Linear Discriminant Functions Statistical Learning Theory & SVMs Ensemble Methods & Boosting Randomized Trees, Forests & Ferns Generative Models (4 weeks) Bayesian Networks Markov Random Fields

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Topics of This Lecture

· Recap: Generalized Linear Discriminants

- · Logistic Regression
 - > Probabilistic discriminative models
 - > Logistic sigmoid (logit function)
 - > Cross-entropy error
 - Gradient descent
 - > Iteratively Reweighted Least Squares
- Note on error functions

• Statistical Learning Theory

- \succ Generalization and overfitting
- Empirical and actual risk
- VC dimension
- Empirical Risk Minimization
- Structural Risk Minimization

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Recap: Linear Discriminant Functions • Basic idea • Directly encode decision boundary • Minimize misclassification probability directly. • Linear discriminant functions y = 0 y > 0weight vector "bias" (= threshold) • w, w_0 define a hyperplane in \mathbb{R}^D . • If a data set can be perfectly classified by a linear discriminant, then we call it linearly separable.

Recap: Extension to Nonlinear Basis Fcts.

Generalization

> Transform vector $\mathbf x$ with M nonlinear basis functions $\phi_i(\mathbf x)$:

$$y_k(\mathbf{x}) = \sum_{j=1}^{M} w_{kj} \phi_j(\mathbf{x}) + w_{k0}$$

Advantages

- > Transformation allows non-linear decision boundaries.
- > By choosing the right ϕ_j , every continuous function can (in principle) be approximated with arbitrary accuracy.

Disadvantage

- The error function can in general no longer be minimized in closed form.
- ⇒ Minimization with Gradient Descent

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Recap: Basis Functions • Generally, we consider models of the following form $y_k(\mathbf{x}) = \sum_{j=0}^M w_{kj}\phi_j(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x})$ • where $\phi_j(\mathbf{x})$ are known as basis functions. • In the simplest case, we use linear basis functions: $\phi_d(\mathbf{x}) = x_d$. • Other popular basis functions | Other popular basis fun

Gradient Descent

· Iterative minimization

- > Start with an initial guess for the parameter values $w_{k\cdot i}^{(0)}$.
- > Move towards a (local) minimum by following the gradient,
- Basic strategies
- "Batch learning"

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

"Sequential updating"
$$\left.w_{kj}^{(\tau+1)}=w_{kj}^{(\tau)}-\eta\left.\frac{\partial E_n(\mathbf{w})}{\partial w_{kj}}\right|_{\mathbf{w}^{(\tau)}}\right|_{\mathbf{w}^{(\tau)}}$$

where
$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

Recap: Gradient Descent

· Example: Quadratic error function

$$E(\mathbf{w}) = \sum_{n=1}^{N} (y(\mathbf{x}_n; \mathbf{w}) - \mathbf{t}_n)^2$$

Sequential updating leads to delta rule (=LMS rule)

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta (y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}) \phi_j(\mathbf{x}_n)$$
$$= w_{kj}^{(\tau)} - \eta \delta_{kn} \phi_j(\mathbf{x}_n)$$

$$\delta_{kn} = y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}$$

⇒ Simply feed back the input data point, weighted by the classification error.

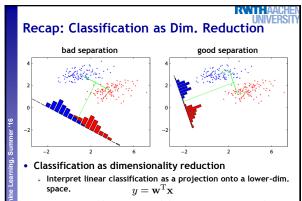
Recap: Gradient Descent

· Cases with differentiable, non-linear activation function

$$y_k(\mathbf{x}) = g(a_k) = g\left(\sum_{j=0}^{M} w_{ki}\phi_j(\mathbf{x}_n)\right)$$

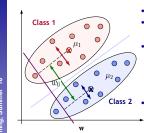
• Gradient descent (again with quadratic error function)

$$\begin{split} \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} &= \frac{\partial g(a_k)}{\partial w_{kj}} \left(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \phi_j(\mathbf{x}_n) \\ w_{kj}^{(\tau+1)} &= w_{kj}^{(\tau)} - \eta \delta_{kn} \phi_j(\mathbf{x}_n) \\ \delta_{kn} &= \frac{\partial g(a_k)}{\partial w_{kj}} \left(y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn} \right) \end{split}$$



 \Rightarrow Learning problem: Try to find the projection vector \mathbf{w} that maximizes class separation.

Recap: Fisher's Linear Discriminant Analysis



- Maximize distance between classes
- Minimize distance within a class

 \mathbf{S}_{B} ... between-class scatter matrix $\mathbf{S}_{\mathit{W}} \dots$ within-class scatter matrix

The optimal solution for w can be obtained as:

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

Classification function:

Classification function:
$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 \mathop{\gtrless}\limits_{\text{Class } 2}^{\text{Class } 1} 0$$
 where $w_0 = -\mathbf{w}^T\mathbf{m}$

Topics of This Lecture

- · Recap: Generalized Linear Discriminants
- Logistic Regression
 - Probabilistic discriminative models
 - Logistic sigmoid (logit function)
 - Cross-entropy error
 - Gradient descent
 - Iteratively Reweighted Least Squares
- Note on error functions
- Statistical Learning Theory
 - Generalization and overfitting Empirical and actual risk
- VC dimension
- **Empirical Risk Minimization**
- Structural Risk Minimization

function

Probabilistic Discriminative Models

· We have seen that we can write

$$p(C_1|\mathbf{x}) = \sigma(a)$$

= $\frac{1}{1 + \exp(-a)}$

· We can obtain the familiar probabilistic model by setting

$$a = \ln \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

Or we can use generalized linear discriminant models

$$a = \mathbf{w}^T \mathbf{x}$$

or
$$a = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

Probabilistic Discriminative Models

In the following, we will consider models of the form

$$p(C_1|\boldsymbol{\phi}) = y(\boldsymbol{\phi}) = \sigma(\mathbf{w}^T \boldsymbol{\phi})$$

with
$$p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

This model is called logistic regression.

Why should we do this? What advantage does such a model have compared to modeling the probabilities?

$$p(\mathcal{C}_1|\boldsymbol{\phi}) \ = \ \frac{p(\boldsymbol{\phi}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\boldsymbol{\phi}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\boldsymbol{\phi}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

· Any ideas?

Comparison

- · Let's look at the number of parameters...
 - > Assume we have an M-dimensional feature space ϕ .
 - And assume we represent $p(\phi | C_k)$ and $p(C_k)$ by Gaussians.
 - > How many parameters do we need?
 - For the means:

 - For the covariances: M(M+1)/2
 - Together with the class priors, this gives M(M+5)/2+1 parameters!
 - > How many parameters do we need for logistic regression?

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = y(\boldsymbol{\phi}) = \sigma(\mathbf{w}^T\boldsymbol{\phi})$$

Just the values of w ⇒ M parameters,

 \Rightarrow For large M, logistic regression has clear advantages!

Logistic Sigmoid

perioder class
$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

Inverse:
$$a = \ln\left(\frac{\sigma}{1-\sigma}\right)$$

Symmetry property:

$$\sigma(-a) = 1 - \sigma(a)$$

Derivative: $\frac{d\sigma}{da} = \sigma(1-\sigma)$

Logistic Regression

- Let's consider a data set $\{\phi_n,t_n\}$ with $n=1,\ldots,N$, where $\phi_n=\phi(\mathbf{x}_n)$ and $t_n\in\{0,1\}$, $\mathbf{t}=(t_1,\ldots,t_N)^T$.
- With $y_n=p(\mathcal{C}_1|\pmb{\phi}_n)$, we can write the likelihood as $p(\mathbf{t}|\mathbf{w})=\prod_{n=1}^Ny_n^{t_n}\left\{1-y_n\right\}^{1-t_n}$

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \left\{ 1 - y_n \right\}^{1 - t_n}$$

· Define the error function as the negative log-likelihood $E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w})$

$$= -\sum_{n=1}^{N} \{t_n \ln y_n + (1-t_n) \ln(1-y_n)\}\$$

> This is the so-called cross-entropy error function.

$$\frac{dy_n}{d\mathbf{w}} = y_n(1 - y_n)\boldsymbol{\phi}_n$$

Gradient of the Error Function
$$y_n = \sigma(\mathbf{w}^T \phi_n)$$
• Error function
$$\frac{dy_n}{d\mathbf{w}} = y_n(1-y_n)\phi_n$$

$$E(\mathbf{w}) = -\sum_{n=1}^N \{t_n \ln y_n + (1-t_n) \ln(1-y_n)\}$$
• Gradient

$$\begin{split} \nabla E(\mathbf{w}) &= -\sum_{n=1}^{N} \left\{ t_n \frac{\frac{d}{d\mathbf{w}} y_n}{y_n} + (1 - t_n) \frac{\frac{d}{d\mathbf{w}} (1 - y_n)}{(1 - y_n)} \right\} \\ &= -\sum_{n=1}^{N} \left\{ t_n \frac{y_n (1 - y_n)}{y_n} \phi_n - (1 - t_n) \frac{y_n (1 - y_n)}{(1 - y_n)} \phi_n \right\} \\ &= -\sum_{n=1}^{N} \left\{ (t_n - t_n y_n - y_n + t_n y_n) \phi_n \right\} \\ &= \sum_{n=1}^{N} (y_n - t_n) \phi_n \end{split}$$

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Gradient of the Error Function

· Gradient for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \boldsymbol{\phi}_n$$

- · Does this look familiar to you?
- This is the same result as for the Delta (=LMS) rule
 - $w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} \eta(y_k(\mathbf{x}_n; \mathbf{w}) t_{kn})\phi_j(\mathbf{x}_n)$
- We can use this to derive a sequential estimation algorithm.
 - However, this will be quite slow...

A More Efficient Iterative Method...

· Second-order Newton-Raphson gradient descent scheme

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \mathbf{H}^{-1} \nabla E(\mathbf{w})$$

where $\mathbf{H} = \nabla \nabla E(\mathbf{w})$ is the Hessian matrix, i.e. the matrix of second derivatives.

- Properties
 - > Local quadratic approximation to the log-likelihood.
 - Faster convergence.

Newton-Raphson for Least-Squares Estimation

· Let's first apply Newton-Raphson to the least-squares error function:

$$\begin{split} E(\mathbf{w}) &= \frac{1}{2} \sum_{n=1}^{N} \left(\mathbf{w}^{T} \boldsymbol{\phi}_{n} - t_{n} \right)^{2} \\ \nabla E(\mathbf{w}) &= \sum_{n=1}^{N} \left(\mathbf{w}^{T} \boldsymbol{\phi}_{n} - t_{n} \right) \boldsymbol{\phi}_{n} = \boldsymbol{\Phi}^{T} \boldsymbol{\Phi} \mathbf{w} - \boldsymbol{\Phi}^{T} \mathbf{t} \\ \mathbf{H} &= \nabla \nabla E(\mathbf{w}) &= \sum_{n=1}^{N} \boldsymbol{\phi}_{n} \boldsymbol{\phi}_{n}^{T} = \boldsymbol{\Phi}^{T} \boldsymbol{\Phi} & \text{where } \boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}_{1}^{T} \\ \vdots \\ \boldsymbol{\phi}_{N}^{T} \end{bmatrix} \end{split}$$

· Resulting update scheme:

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T \mathbf{\Phi})^{-1} (\mathbf{\Phi}^T \mathbf{\Phi} \mathbf{w}^{(\tau)} - \mathbf{\Phi}^T \mathbf{t})$$
$$= (\mathbf{\Phi}^T \mathbf{\Phi})^{-1} \mathbf{\Phi}^T \mathbf{t} \qquad \text{Closed-form solution}$$

Closed-form solution!

Newton-Raphson for Logistic Regression

· Now, let's try Newton-Raphson on the cross-entropy error function:

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right\}$$

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \phi_n = \mathbf{\Phi}^T(\mathbf{y} - \mathbf{t})$$

 $\mathbf{H} = \nabla \nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n (1 - y_n) \phi_n \phi_n^T = \mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi}$

where ${\bf R}$ is an $N{\times}N$ diagonal matrix with $R_{nn}=y_n(1-y_n)$.

 \Rightarrow The Hessian is no longer constant, but depends on w through the weighting matrix ${f R}.$

Iteratively Reweighted Least Squares

Update equations

$$\begin{split} \mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi})^{-1} \mathbf{\Phi}^T (\mathbf{y} - \mathbf{t}) \\ &= (\mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi})^{-1} \left\{ \mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi} \mathbf{w}^{(\tau)} - \mathbf{\Phi}^T (\mathbf{y} - \mathbf{t}) \right\} \\ &= (\mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi})^{-1} \mathbf{\Phi}^T \mathbf{R} \mathbf{z} \end{split}$$

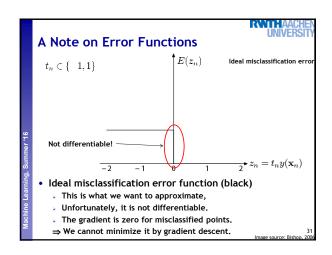
with
$$\mathbf{z} = \mathbf{\Phi} \mathbf{w}^{(au)} - \mathbf{R}^{-1} (\mathbf{y} - \mathbf{t})$$

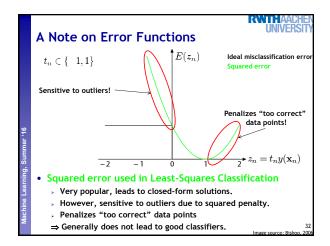
- · Again very similar form (normal equations)
 - > But now with non-constant weighing matrix ${f R}$ (depends on ${f w}$).
 - > Need to apply normal equations iteratively.
 - ⇒ Iteratively Reweighted Least-Squares (IRLS)

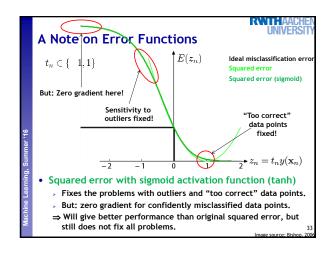
Summary: Logistic Regression

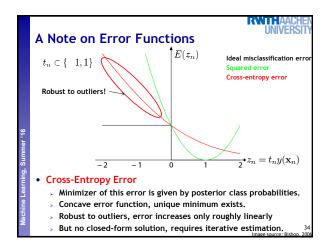
- Properties
 - \triangleright Directly represent posterior distribution $p(\phi \mid C_b)$
 - Requires fewer parameters than modeling the likelihood + prior.
 - Very often used in statistics.
 - > It can be shown that the cross-entropy error function is concave
 - Optimization leads to unique minimum
 - But no closed-form solution exists
 - Iterative optimization (IRLS)
 - > Both online and batch optimizations exist There is a multi-class version described in (Bishop Ch.4.3.4).
- Caveat
 - Logistic regression tends to systematically overestimate odds ratios when the sample size is less than ~500.

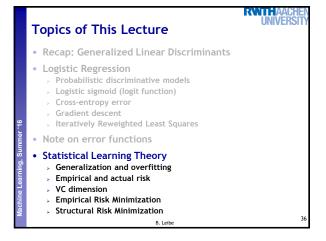
Topics of This Lecture Recap: Generalized Linear Discriminants Logistic Regression Probabilistic discriminative models Logistic sigmoid (logit function) Cross-entropy error Gradient descent Iteratively Reweighted Least Squares Note on error functions Statistical Learning Theory Generalization and overfitting Empirical and actual risk VC dimension Empirical Risk Minimization Structural Risk Minimization B. Leibe

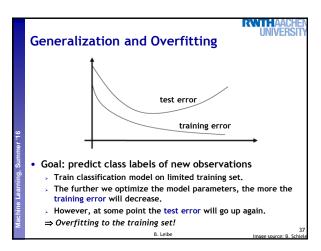












Example: Linearly Separable Data • Overfitting is often a problem with linearly separable data • Which of the many possible decision boundaries is correct? • All of them have zero error on the training set... • However, they will most likely result in different predictions on novel test data. ⇒ Different generalization performance • How to select the classifier with the best generalization performance?

A Broader View on Statistical Learning • Formal treatment: Statistical Learning Theory • Supervised learning • Environment: assumed stationary. • I.e. the data \mathbf{x} have an unknown but fixed probability density $p_X(\mathbf{x})$ • Teacher: specifies for each data point \mathbf{x} the desired classification y (where y may be subject to noise). $y = g(\mathbf{x}, \nu)$ with noise ν • Learning machine: represented by class of functions, which produce for each \mathbf{x} an output y: $y = f(\mathbf{x}; \alpha)$ with parameters α

Statistical Learning Theory • Supervised learning (from the learning machine's view) • Selection of a specific function $f(\mathbf{x};\alpha)$ • Given: training examples $\{(\mathbf{x}_i,y_i)\}_{i=1}^N$ • Goal: the desired response y shall be approximated optimally. • Measuring the optimality • Loss function $L(y,f(\mathbf{x};\alpha))$ • Example: quadratic loss $L(y,f(\mathbf{x};\alpha)) = (y-f(\mathbf{x};\alpha))^2$

Risk • Measuring the "optimality" • Measure the optimality by the risk (= expected loss). • Difficulty: how should the risk be estimated? • Practical way • Empirical risk (measured on the training/validation set) $R_{emp}(\alpha) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(\mathbf{x}_i; \alpha))$ • Example: quadratic loss function $R_{emp}(\alpha) = \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i; \alpha))^2$

	Risk	ΙΤΥ
	However, what we're really interested in is Actual risk (= Expected risk)	
	$R(\alpha) = \int L(y, f(\mathbf{x}; \alpha)) dP_{X,Y}(\mathbf{x}, y)$	
	, $P_{X,Y}(\mathbf{x},y)$ is the probability distribution of (\mathbf{x},y) .	
anumer	$P_{X,Y}(\mathbf{x},y)$ is fixed, but typically unknown. \Rightarrow In general, we can't compute the actual risk directly!	
irning,	\succ The expected risk is the expectation of the error on \emph{all} data.	
cuine Lea	. I.e., it is the expected value of the generalization error.	
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- Actual risk Advantage: measure for the generalization ability
 - ightarrow Disadvantage: in general, we don't know $P_{X,Y}(\mathbf{x},y)$
- Empirical risk
 - > Disadvantage: no direct measure of the generalization ability
 - Advantage: does not depend on $P_{X,Y}(\mathbf{x},y)$
 - > We typically know learning algorithms which minimize the empirical risk.
- ⇒ Strong interest in connection between both types of risk

Statistical Learning Theory

- Idea
 - Compute an upper bound on the actual risk based on the empirical risk

$$R(\alpha) \cdot R_{emp}(\alpha) + \epsilon(N, p^*, h)$$

- where
- N: number of training examples
 - p^* : probability that the bound is correct
 - h: capacity of the learning machine ("VC-dimension")
- · Side note:
 - (This idea of specifying a bound that only holds with a certain probability is explored in a branch of learning theory called "Probably Approximately Correct" or PAC Learning).

VC Dimension

- · Vapnik-Chervonenkis dimension
 - > Measure for the capacity of a learning machine.
- Formal definition:
 - If a given set of ℓ points can be labeled in all possible 2^{ℓ} ways, and for each labeling, a member of the set $\{f(\alpha)\}$ can be found which correctly assigns those labels, we say that the set of points is shattered by the set of functions.
 - ightarrow The VC dimension for the set of functions $\{f(lpha)\}$ is defined as the maximum number of training points that can be shattered by $\{f(\alpha)\}$.

VC Dimension

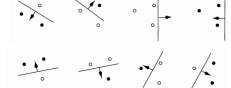
- · Interpretation as a two-player game
 - > Opponent's turn: He says a number N.
 - We specify a set of N points $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. Our turn:
 - > Opponent's turn: He gives us a labeling $\{\mathbf{x}_1, ..., \mathbf{x}_N\} \in \{0,1\}^N$
 - Our turn: We specify a function $f(\alpha)$ which correctly classifies all ${\cal N}$ points.

 \Rightarrow If we can do that for all 2^N possible labelings, then the VC dimension is at least N.

VC Dimension

Example

- - > The VC dimension of all oriented lines in \mathbb{R}^2 is 3.
 - 1. Shattering 3 points with an oriented line:



- 2. More difficult to show; it is not possible to shatter 4 points (XOR)...
- More general: the VC dimension of all hyperplanes in \mathbb{R}^n is $n{+}1$.

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VC Dimension

- · Intuitive feeling (unfortunately wrong)
 - The VC dimension has a direct connection with the number of parameters.
- Counterexample

$$f(x;\alpha) = g(\sin(\alpha x))$$
$$g(x) = \begin{cases} 1, & x > 0 \\ -1, & x \cdot 0 \end{cases}$$

- Just a single parameter α .
- Infinite VC dimension
 - $x_i = 10^{-i}, \quad i = 1, \dots, \ell$ Proof: Choose

Upper Bound on the Risk $\begin{tabular}{ll} & \textbf{University} \\ & \textbf{Important result (Vapnik 1979, 1995)} \\ & \textbf{With probability } & \textbf{(1-η), the following bound holds} \\ & R(\alpha) \cdot & R_{emp}(\alpha) + \sqrt{\frac{h(\log(2N/h)+1)-\log(\eta/4)}{N}} \\ & \textbf{"VC confidence"} \\ & \textbf{This bound is independent of } P_{X,Y}(\mathbf{x},y)! \\ & \textbf{Typically, we cannot compute the left-hand side (the actual risk)} \\ & \textbf{If we know } h \text{ (the VC dimension), we can however easily compute the risk bound} \\ \end{tabular}$

 $R(lpha) \cdot R_{emp}(lpha) + \epsilon(N,p^*,h)$

