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Machine Learning - Lecture 7

Statistical Learning Theory

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Many slides adapted from B. Schiele

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

- 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 $y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \mathbf{x} + w_0$ weight 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

 \succ Transform vector ${\bf x}$ with M nonlinear basis functions $\phi_i({\bf x})$:

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

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.

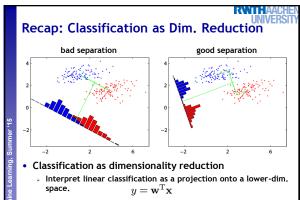
Recap: Gradient Descent

· Cases with differentiable, non-linear activation function

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

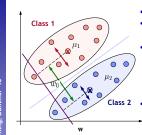
• Gradient descent (again with quadratic error function)

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



 \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:
$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0 \mathop{\gtrsim}\limits_{\mathrm{Class}}^{\mathrm{Class}} \mathop{>}\limits_{0}^{1} 0$$
 where $w_0 = -\mathbf{w}^T \mathbf{m}$

Note on error functions Statistical Learning Theory Generalization and overfitting Empirical and actual risk

VC dimension **Empirical Risk Minimization**

Topics of This Lecture

Probabilistic discriminative models Logistic sigmoid (logit function) Cross-entropy error

Iteratively Reweighted Least Squares

• Logistic Regression

Gradient descent

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

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

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

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

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

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}^{M} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}\$$

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

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

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

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

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:

$$\begin{split} \mathbf{w}^{(\bar{\tau}+1)} &= \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}(\mathbf{\Phi}^T\mathbf{\Phi}\mathbf{w}^{(\tau)} - \mathbf{\Phi}^T\mathbf{t}) \\ &= (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{t} & \text{Closed-form solution.} \end{split}$$

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

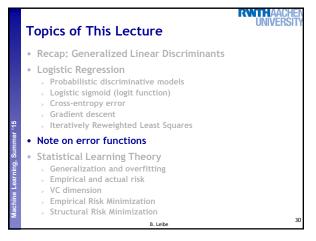
$$\begin{split} \mathbf{w}^{(\tau+1)} &= \mathbf{w}^{(\tau)} - (\mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi})^{-1} \mathbf{\Phi}^T (\mathbf{y} - \mathbf{t}) \\ &= (\mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi})^{-1} \left\{ \mathbf{\Phi}^T \mathbf{R} \mathbf{\Phi} \mathbf{w}^{(\tau)} - \mathbf{\Phi}^T (\mathbf{y}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

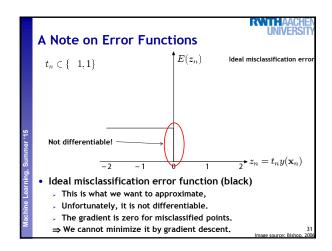
with
$$\mathbf{z} = \mathbf{\Phi} \mathbf{w}^{(\tau)} - \mathbf{R}^{-1} (\mathbf{v} - \mathbf{t})$$

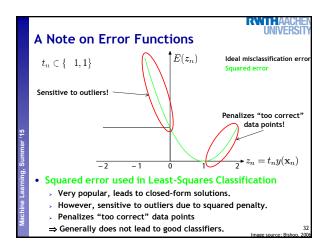
- · Again very similar form (normal equations)
 - > But now with non-constant weighing matrix ${f R}$ (depends on ${f w}$).
 - > Need to apply normal equations iteratively.
 - ⇒ Iteratively Reweighted Least-Squares (IRLS)

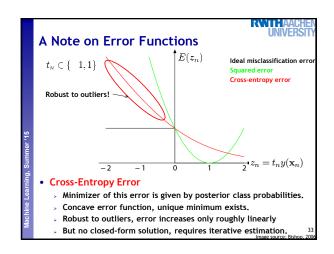
Summary: Logistic Regression

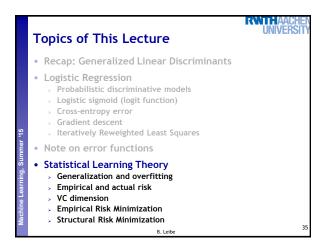
- Properties
 - \triangleright Directly represent posterior distribution $p(\phi \mid C_l)$
 - Requires fewer parameters than modeling the likelihood + prior.
 - Very often used in statistics.
 - > It can be shown that the cross-entropy error function is concave
 - Optimization leads to unique minimum
 - 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.

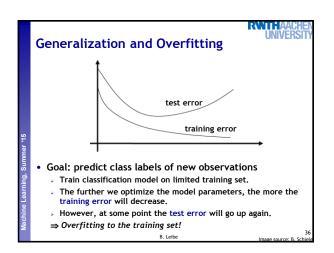












Example: Linearly Separable Data

- 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?

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A Broader View on Statistical Learning

- Formal treatment: Statistical Learning Theory
- Supervised learning
 - > Environment; assumed stationary.
 - > I.e. the data ${f x}$ have an unknown but fixed probability density

$$p_X(\mathbf{x})$$

> Teacher: specifies for each data point ${\bf x}$ 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 ${\bf x}$ an output y:

$$y=f(\mathbf{x}; \alpha)$$
 with parameters α

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Statistical Learning Theory

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

$$L(y, f(\mathbf{x}; \alpha))$$

> Example: quadratic loss

$$L(y, f(\mathbf{x}; \alpha)) = (y - f(\mathbf{x}; \alpha))^2$$

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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

$$R_{emp}(lpha) = rac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i; lpha))^2$$

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Risk

- · 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) .
- $P_{X,Y}(\mathbf{x},y)$ is fixed, but typically unknown.
- ⇒ In general, we can't compute the actual risk directly!
- > The expected risk is the expectation of the error on all data.
- \succ I.e., it is the expected value of the generalization error.

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Summary: Risk

- Actual risk
 - Advantage: measure for the generalization ability
 - > Disadvantage: in general, we don't know $P_{X,Y}(\mathbf{x},y)$
- Empirical risk
 - > Disadvantage: no direct measure of the generalization ability
 - ightarrow 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

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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).

Slide adapted from Bernt Schiele

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.
 - > The VC dimension for the set of functions $\{f(\alpha)\}$ is defined as the maximum number of training points that can be shattered by $\{f(\alpha)\}$.

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VC Dimension

- · Interpretation as a two-player game

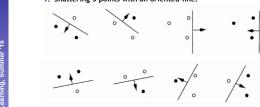
 - **Our turn:** We specify a set of N points $\{\mathbf{x}_1, ..., \mathbf{x}_N\}$.
 - \succ Opponent's turn: He gives us a labeling $\{\mathbf{x}_{_{1}},\!\dots,\!\mathbf{x}_{N}\}\!\in\{0,\!1\}^{N}$
 - \rightarrow Our turn: We specify a function $f(\alpha)$ which correctly
 - classifies all N points.
 - \Rightarrow If we can do that for all 2^N possible labelings, then the VC dimension is at least N.

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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)...
- ightarrow More general; the VC dimension of all hyperplanes in \mathbb{R}^n is $n{+}1$,

ide adanted from Bernt Schiele B. Leibe Image source: C. Burges. 199

VC Dimension

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

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

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

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

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Upper Bound on the Risk

- · Important result (Vapnik 1979, 1995)
 - \rightarrow With probability $(1-\eta)$, the following bound holds

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

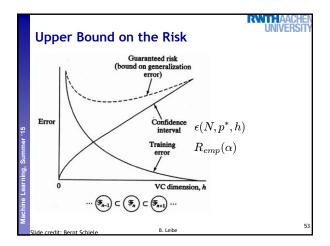
"VC confidence"

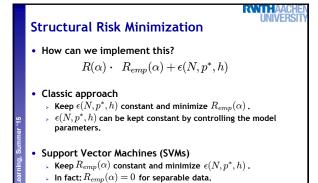
- This bound is independent of $P_{X,Y}(\mathbf{x},y)$!
- > Typically, we cannot compute the left-hand side (the actual risk)
- $\ \ \, \text{If we know} \, \, h \, \, \text{(the VC dimension), we can however easily compute the risk bound}$

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

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Control $\epsilon(N,p^*,h)$ by adapting the VC dimension (controlling the "capacity" of the classifier).

References and Further Reading

• More information on SVMs can be found in Chapter 7.1 of Bishop's book.

Christopher M. Bishop Pattern Recognition and Machine Learning Springer, 2006

• Additional information about Statistical Learning Theory and a more in-depth introduction to SVMs are available in the following tutorial:

• C. Burges, A Tutorial on Support Vector Machines for Pattern Recognition, Data Mining and Knowledge Discovery, Vol. 2(2), pp. 121-167 1998.