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Machine Learning – Lecture 9

Model Combination

13.11.2017

Bastian Leibe RWTH Aachen http://www.vision.rwth-aachen.de

leibe@vision.rwth-aachen.de

Course Outline Fundamentals Bayes Decision Theory Probability Density Estimation Classification Approaches Linear Discriminants Support Vector Machines Ensemble Methods & Boosting Randomized Trees, Forests & Ferns Deep Learning Foundations Convolutional Neural Networks Recurrent Neural Networks

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Topics of This Lecture

- Recap: Nonlinear Support Vector Machines
- Analysis
- Error function
- Applications
- Ensembles of classifiers
 - Bagging
 - Bayesian Model Averaging
- AdaBoost
 - Intuition
 - Algorithm
 - Analysis
 - Extensions

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Recap: Support Vector Machine (SVM)

Basic idea

- The SVM tries to find a classifier which maximizes the margin between pos. and neg. data points.
- Up to now: consider linear classifiers



- Formulation as a convex optimization problem
 - Find the hyperplane satisfying

$$\underset{\mathbf{w},b}{\operatorname{arg\,min}} \frac{1}{2} \|\mathbf{w}\|^2$$

under the constraints

$$t_n(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n + b) \ge 1 \quad \forall n$$

based on training data points \mathbf{x}_n and target values $t_n \in \{-1,1\}$

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Recap: SVM – Dual Formulation

Maximize

$$L_d(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m(\mathbf{x}_m^{\mathsf{T}} \mathbf{x}_n)$$

under the conditions

$$a_n \geq 0 \quad \forall n$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

- Comparison
 - > L_d is equivalent to the primal form L_p , but only depends on a_n .
 - L_p scales with $\mathcal{O}(D^3)$.
 - L_d scales with $\mathcal{O}(N^3)$ in practice between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.

Slide adapted from Bernt Schiele

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Recap: SVM for Non-Separable Data

- Slack variables
 - > One slack variable $\xi_n \ge 0$ for each training data point.
- Interpretation
 - > $\xi_n = 0$ for points that are on the correct side of the margin.
 - > $\xi_n = |t_n y(\mathbf{x}_n)|$ for all other points.



Point on decision boundary: $\xi_n = 1$

 $\begin{array}{c} \text{Misclassified point:} \\ \xi_n > 1 \end{array}$

- > We do not have to set the slack variables ourselves!
- ⇒ They are jointly optimized together with w.

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Recap: SVM - New Dual Formulation

• New SVM Dual: Maximize
$$L_d(\mathbf{a}) = \sum_{n=1}^N a_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N a_n a_m t_n t_m(\mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n)$$

under the conditions

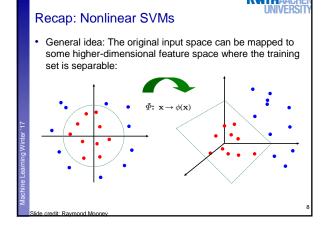
$$0 \cdot a_n \cdot C$$

This is all that changed!

$$\sum_{n=1}^{N} a_n t_n = 0$$

This is again a quadratic programming problem

⇒ Solve as before...



Recap: The Kernel Trick

Important observation

 $\phi(\mathbf{x})$ only appears in the form of dot products $\phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{y})$:

$$\begin{split} y(\mathbf{x}) &= & \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}) + b \\ &= & \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)^{\mathrm{T}} \phi(\mathbf{x}) + b \end{split}$$

> Define a so-called kernel function $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^\mathsf{T} \phi(\mathbf{y})$.

> Now, in place of the dot product, use the kernel instead:

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$

> The kernel function implicitly maps the data to the higherdimensional space (without having to compute $\phi(\mathbf{x})$ explicitly)!

Nonlinear SVM - Dual Formulation

• SVM Dual: Maximize
$$L_d(\mathbf{a}) = \sum_{n=1}^N a_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N a_n a_m t_n t_m \frac{\mathbf{k}(\mathbf{x}_m, \mathbf{x}_n)}{\mathbf{k}(\mathbf{x}_m, \mathbf{x}_n)}$$

under the conditions

$$0 \cdot a_n \cdot C$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

· Classify new data points using

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n \mathbf{k}(\mathbf{x}_n, \mathbf{x}) + b$$

Summary: SVMs

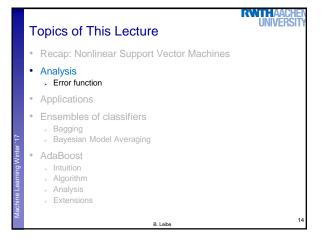
Properties

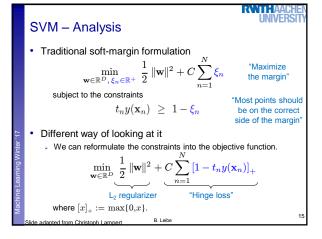
- > Empirically, SVMs work very, very well.
- > SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.
- > SVM techniques have been applied to a variety of other tasks
 - e.g. SV Regression, One-class SVMs. ..
- The kernel trick has been used for a wide variety of applications. It can be applied wherever dot products are in use
 - e.g. Kernel PCA, kernel FLD, ..
 - Good overview, software, and tutorials available on http://www.kernel-

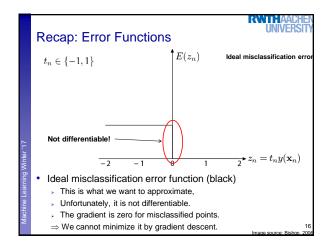
Summary: SVMs

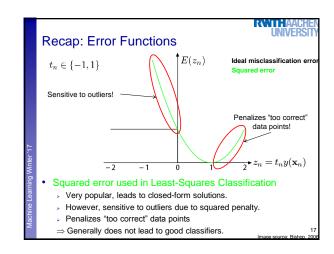
- Limitations
 - How to select the right kernel?
 - Best practice guidelines are available for many applications
 - How to select the kernel parameters?
 - (Massive) cross-validation.
 - Usually, several parameters are optimized together in a grid search.
 - > Solving the quadratic programming problem
 - Standard QP solvers do not perform too well on SVM task.
 - Dedicated methods have been developed for this, e.g. SMO.
 - Speed of evaluation
 - Evaluating y(x) scales linearly in the number of SVs.
 - Too expensive if we have a large number of support vectors. ⇒ There are techniques to reduce the effective SV set.
 - Training for very large datasets (millions of data points)

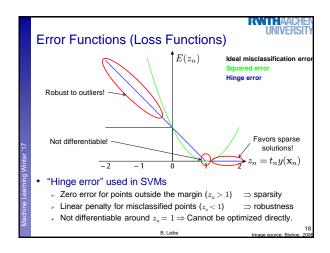
- Stochastic gradient descent and other approximations can be used

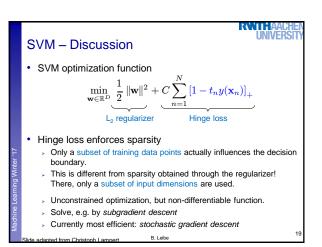


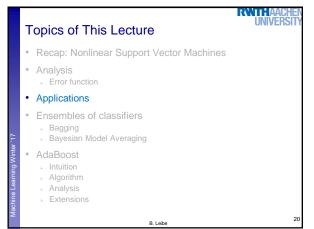


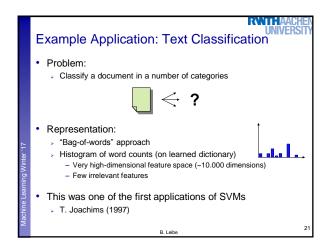


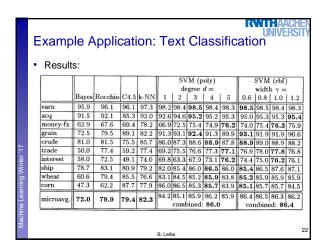


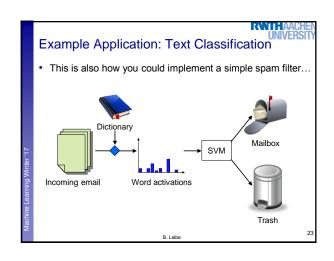


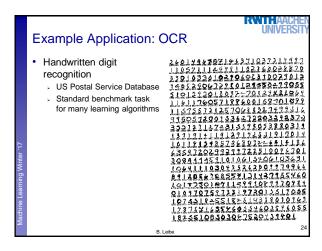


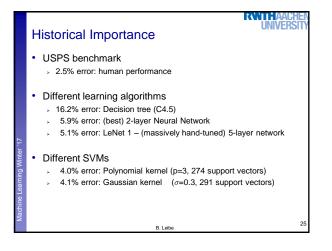


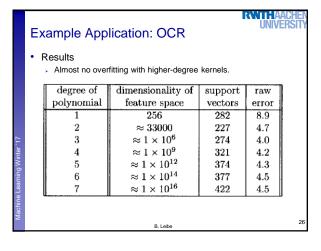


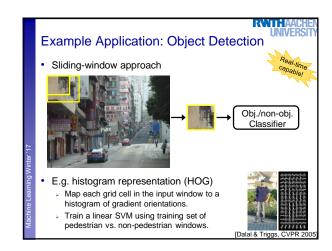






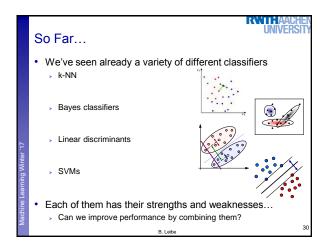


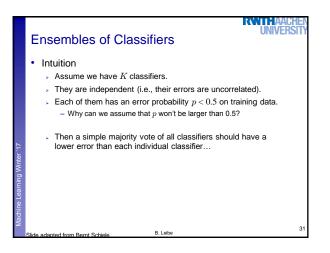














Constructing Ensembles

- · How do we get different classifiers?
 - > Simplest case: train same classifier on different data.
 - > But... where shall we get this additional data from?
 - Recall: training data is very expensive!
- · Idea: Subsample the training data
 - Reuse the same training algorithm several times on different subsets of the training data.
- · Well-suited for "unstable" learning algorithms
 - Unstable: small differences in training data can produce very different classifiers
 - E.g., Decision trees, neural networks, rule learning algorithms,...

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- Stable learning algorithms
 - E.g., Nearest neighbor, linear regression, SVMs,...

Constructing Ensembles

- Bagging = "Bootstrap aggregation" (Breiman 1996)
 - ightarrow In each run of the training algorithm, randomly select M samples from the full set of N training data points.
 - \sim If M=N, then on average, 63.2% of the training points will be represented. The rest are duplicates.
- Injecting randomness
 - Many (iterative) learning algorithms need a random initialization (e.g. k-means, EM)
 - Perform mutliple runs of the learning algorithm with different random initializations.

Slide adapted from Bern

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Bayesian Model Averaging

- Model Averaging
 - Suppose we have H different models h = 1,...,H with prior probabilities p(h).
 - Construct the marginal distribution over the data set

$$p(\mathbf{X}) = \sum_{h=1}^{H} p(\mathbf{X}|h)p(h)$$

Interpretation

- Just one model is responsible for generating the entire data set.
- \rightarrow The probability distribution over h just reflects our uncertainty which model that is.
- As the size of the data set increases, this uncertainty reduces, and $p(\mathbf{X}|h)$ becomes focused on just one of the models.

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Note the Different Interpretations!

- Model Combination (e.g., Mixtures of Gaussians)
 - > Different data points generated by different model components.
 - Uncertainty is about which component created which data point.
 - \Rightarrow One latent variable \mathbf{z}_n for each data point:

$$p(\mathbf{X}) = \prod_{n=1}^{N} p(\mathbf{x}_n) = \prod_{n=1}^{N} \sum_{\mathbf{z}_n} p(\mathbf{x}_n, \mathbf{z}_n)$$

- Bayesian Model Averaging
 - > The whole data set is generated by a single model.
 - > Uncertainty is about which model was responsible.
 - ⇒ One latent variable **z** for the entire data set:

$$p(\mathbf{X}) = \sum_{\mathbf{z}} p(\mathbf{X}, \mathbf{z})$$
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Model Averaging: Expected Error

- Combine M predictors $y_m(\mathbf{x})$ for target output $h(\mathbf{x})$.
 - E.g. each trained on a different bootstrap data set by bagging.
 - > The committee prediction is given by

$$y_{COM}(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x})$$

> The output can be written as the true value plus some error.

$$y(\mathbf{x}) = h(\mathbf{x}) + \epsilon(\mathbf{x})$$

> Thus, the expected sum-of-squares error takes the form

$$\mathbb{E}_{\mathbf{x}} = \left[\left\{ y_m(\mathbf{x}) - h(\mathbf{x}) \right\}^2 \right] = \mathbb{E}_{\mathbf{x}} \left[\epsilon_m(\mathbf{x})^2 \right]$$

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Model Averaging: Expected Error

• Average error of individual models

$$\mathbb{E}_{AV} = \frac{1}{M} \sum_{m=1}^{M} \mathbb{E}_{\mathbf{x}} \left[\epsilon_m(\mathbf{x})^2 \right]$$

Average error of committee

$$\mathbb{E}_{COM} = \mathbb{E}_{\mathbf{x}} \Bigg[\left\{ \frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x}) - h(\mathbf{x}) \right\}^2 \Bigg] = \mathbb{E}_{\mathbf{x}} \Bigg[\left\{ \frac{1}{M} \sum_{m=1}^{M} \epsilon_m(\mathbf{x}) \right\}^2$$

Assumptions

- Figure Errors have zero mean: $\mathbb{E}_{\mathbf{x}}\left[\epsilon_{m}(\mathbf{x})
 ight]=0$
- ${\mathbb E}_{\mathbf x}\left[\epsilon_m({\mathbf x})\epsilon_j({\mathbf x})
 ight]=0$

Then:

$$\mathbb{E}_{COM} = \frac{1}{M} \mathbb{E}_{AV}$$

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Model Averaging: Expected Error · Average error of committee

$$\mathbb{E}_{COM} = \frac{1}{M} \mathbb{E}_{AV}$$

- > This suggests that the average error of a model can be reduced by a factor of M simply by averaging M versions of the model!
- » Spectacular indeed...
- > This sounds almost too good to be true...

And it is... Can you see where the problem is?

- > Unfortunately, this result depends on the assumption that the errors are all uncorrelated.
- > In practice, they will typically be highly correlated.
- > Still, it can be shown that

$$\mathbb{E}_{COM} \cdot \mathbb{E}_{AV}$$

AdaBoost – "Adaptive Boosting"

 Main idea [Freund & Schapire, 1996]

- Iteratively select an ensemble of component classifiers
 - > After each iteration, reweight misclassified training examples.
 - Increase the chance of being selected in a sampled training set.
 - Or increase the misclassification cost when training on the full set.

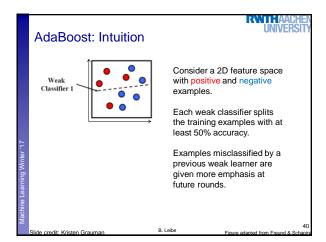
Components

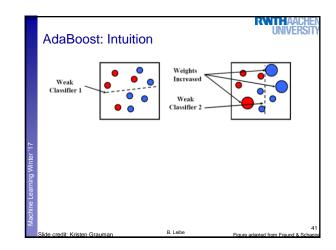
- $h_m(\mathbf{x})$: "weak" or base classifier
 - Condition: <50% training error over any distribution
- $\succ H(\mathbf{x})$: "strong" or final classifier

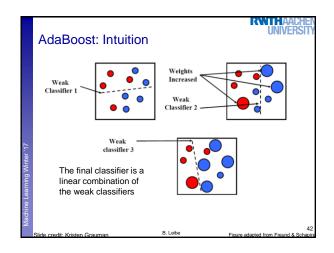
AdaBoost:

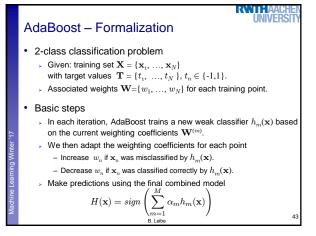
Construct a strong classifier as a thresholded linear combination of the weighted weak classifiers:

$$H(\mathbf{x}) = sign\left(\sum_{m=1}^{M} lpha_m h_m(\mathbf{x})
ight)$$









AdaBoost - Algorithm

- 1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ or n = 1,...,N.
- 2. For m = 1,...,M iterations
 - a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function

$$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n) \qquad I(A) = \begin{cases} 1, & \text{if } A \text{ is true} \\ 0, & \text{else} \end{cases}$$

b) Estimate the weighted error of this classifier on
$$\mathbf{X}$$
:
$$\epsilon_m = \frac{\sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^N w_n^{(m)}}$$
 c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:

$$\alpha_m = ?$$

d) Update the weighting coefficients:

$$w_n^{(m+1)} = ?$$

How should we do this exactly?

AdaBoost – Historical Development

- Originally motivated by Statistical Learning Theory
 - AdaBoost was introduced in 1996 by Freund & Schapire.
 - It was empirically observed that AdaBoost often tends not to overfit. (Breiman 96, Cortes & Drucker 97, etc.)
 - As a result, the margin theory (Schapire et al. 98) developed, which is based on loose generalization bounds.
 - Note: margin for boosting is not the same as margin for SVM.
 - A bit like retrofitting the theory...
- However, those bounds are too loose to be of practical value.
- Different explanation (Friedman, Hastie, Tibshirani, 2000)
- Interpretation as sequential minimization of an exponential error function ("Forward Stagewise Additive Modeling").
- Explains why boosting works well.
- > Improvements possible by altering the error function.

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AdaBoost – Minimizing Exponential Error

Exponential error function

$$E = \sum_{n=1}^{N} \exp\left\{-t_n f_m(\mathbf{x}_n)\right\}$$

» where $f_m(\mathbf{x})$ is a classifier defined as a linear combination of base

$$f_m(\mathbf{x}) = \frac{1}{2} \sum_{l=1}^m \alpha_l h_l(\mathbf{x})$$

- Goal
 - ightarrow Minimize E with respect to both the weighting coefficients $lpha_l$ and the parameters of the base classifiers $h_l(\mathbf{x})$.

AdaBoost - Minimizing Exponential Error

- Sequential Minimization
 - Suppose that the base classifiers $h_1(\mathbf{x}), \dots, h_{m-1}(\mathbf{x})$ and their coefficients $\alpha_1, ..., \alpha_{m-1}$ are fixed.
 - \Rightarrow Only minimize with respect to α_m and $h_m(\mathbf{x})$.

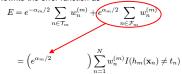
$$E = \sum_{n=1}^{N} \exp\left\{-t_n f_m(\mathbf{x}_n)\right\} \quad \text{with} \quad f_m(\mathbf{x}) = \frac{1}{2} \sum_{l=1}^{m} \alpha_l h_l(\mathbf{x})$$

$$= \sum_{n=1}^{N} \exp\left\{-t_n f_{m-1}(\mathbf{x}_n) - \frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}$$

$$= \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}$$

AdaBoost - Minimizing Exponential Error

- $E = \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}$
- Observation:
 - Correctly classified points: $t_n h_m(\mathbf{x}_n) = +1$
- \Rightarrow collect in \mathcal{T}
- Misclassified points:



AdaBoost – Minimizing Exponential Error $E = \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2}t_n \alpha_m h_m(\mathbf{x}_n)\right\}$ Observation: Correctly classified points: t_nh_m(x_n) = +1 \Rightarrow collect in \mathcal{T} Misclassified points: Rewrite the error function as $= \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$

AdaBoost – Minimizing Exponential Error

• Minimize with respect to $h_m(\mathbf{x})$: $\frac{\partial E}{\partial h_m(\mathbf{x}_n)} \stackrel{!}{=} 0$

$$E = \underbrace{\left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right)}_{n=1} \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$
= const.

 \Rightarrow This is equivalent to minimizing

$$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

(our weighted error function from step 2a) of the algorithm)

⇒ We're on the right track. Let's continue...

AdaBoost – Minimizing Exponential Error • Minimize with respect to α_m : $\frac{\partial E}{\partial \alpha_m} \stackrel{!}{=} 0$ $E = \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$ $\left(\frac{1}{p} e^{\alpha_m/2} + \frac{1}{p} e^{-\alpha_m/2} \right) \sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) \quad \stackrel{!}{=} \quad \frac{1}{p} e^{-\alpha_m/2} \sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n)$ \Rightarrow Update for the α coefficients:

AdaBoost - Minimizing Exponential Error

· Remaining step: update the weights

Recall that

This becomes
$$w_n^{(m+1)}$$

in the next iteration.

> Therefore

$$w_n^{(m+1)} = w_n^{(m)} \exp\left\{-\frac{1}{2}t_n\alpha_m h_m(\mathbf{x}_n)\right\}$$

$$= \dots$$

$$= w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\}$$

⇒ Update for the weight coefficients.

AdaBoost - Final Algorithm

- 1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ or n = 1,...,N.
- **2.** For m = 1,...,M iterations
 - a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function

$$J_m = \sum_{n=0}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

b) Estimate the weighted error of this classifier on X:

$$\epsilon_m = \frac{\sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^N w_n^{(m)}}$$

c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:

weighting coefficient for
$$lpha_m = \ln \left\{ rac{1 - \epsilon_m}{\epsilon_m}
ight\}$$

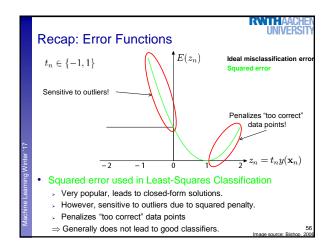
d) Update the weighting coefficients:

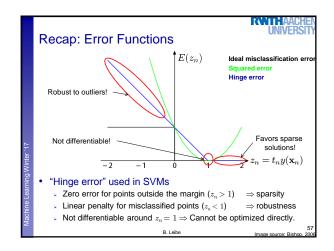
$$w_n^{(m+1)} = w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\}$$

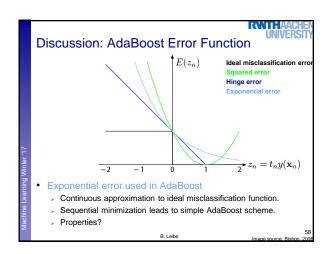
AdaBoost - Analysis

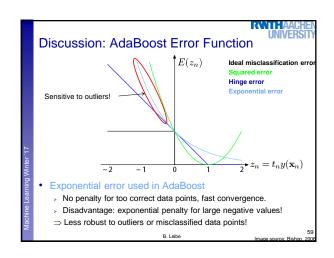
- Result of this derivation
 - We now know that AdaBoost minimizes an exponential error function in a sequential fashion.
 - > This allows us to analyze AdaBoost's behavior in more detail.
 - In particular, we can see how robust it is to outlier data points.

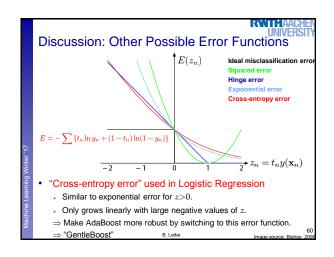
Recap: Error Functions $E(z_n)$ Ideal misclassification erro $t_n \in \{-1, 1\}$ Not differentiable! $z_n = t_n y(\mathbf{x}_n)$ Ideal misclassification error function (black) > This is what we want to approximate, > Unfortunately, it is not differentiable. The gradient is zero for misclassified points. ⇒ We cannot minimize it by gradient descent.

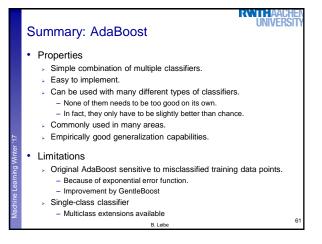












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References and Further Reading

 More information on Classifier Combination and Boosting can be found in Chapters 14.1-14.3 of Bishop's book.

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



- A more in-depth discussion of the statistical interpretation of AdaBoost is available in the following paper:
 - J. Friedman, T. Hastie, R. Tibshirani, <u>Additive Logistic Regression: a Statistical View of Boosting</u>, *The Annals of Statistics*, Vol. 38(2), pages 337-374, 2000.

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