

Machine Learning – Lecture 10

AdaBoost

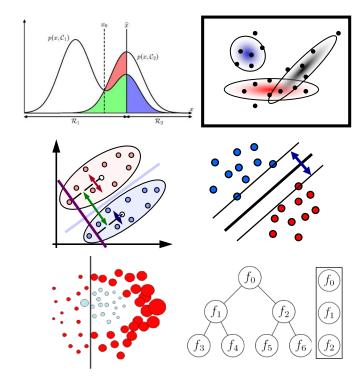
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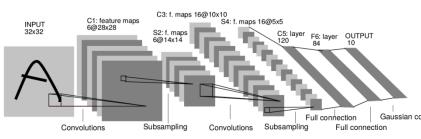
Bastian Leibe RWTH Aachen http://www.vision.rwth-aachen.de

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







Topics of This Lecture

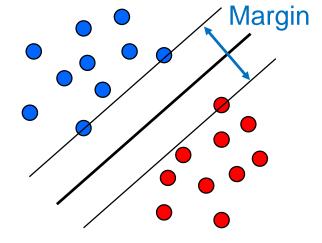
- Recap: Nonlinear Support Vector Machines
- Ensembles of classifiers
 - Bagging
 - Bayesian Model Averaging
- AdaBoost
 - Intuition
 - Algorithm
 - Analysis
 - Extensions

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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

$$\mathbf{w}^{\mathrm{T}}\mathbf{x} + b = 0$$



- 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

 $t_n \in \{-1, 1\}$



Recap: SVM – Dual Formulation

• Maximize

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

under the conditions

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

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

Comparison

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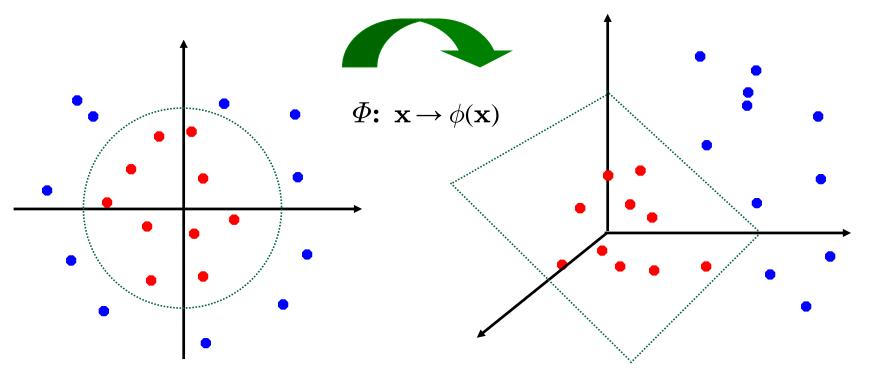
- > L_d is equivalent to the primal form L_p , but only depends on a_n .
- > L_p scales with $\mathcal{O}(D^3)$.
- > L_d scales with $\mathcal{O}(N^3)$ in practice between $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$.

Slide adapted from Bernt Schiele



Recap: Nonlinear SVMs

 General idea: The original input space can be mapped to some higher-dimensional feature space where the training set is separable:





Recap: The Kernel Trick

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

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

- > 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)!

Recap: Nonlinear SVM – Dual Formulation

• SVM Dual: Maximize

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

under the conditions

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

Classify new data points using

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



Recap: SVM Loss Function

Traditional soft-margin formulation

$$\min_{\mathbf{w}\in\mathbb{R}^{D},\,\boldsymbol{\xi}_{n}\in\mathbb{R}^{+}} \frac{1}{2} \|\mathbf{w}\|^{2} + C\sum_{n=1}^{N} \boldsymbol{\xi}_{n}$$

λT

"Maximize the margin"

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \boldsymbol{\xi}_n$$

"Most points should be on the correct side of the margin"

- Different way of looking at it
 - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w} \in \mathbb{R}^{D}} \underbrace{\frac{1}{2} \|\mathbf{w}\|^{2}}_{\mathbf{L}_{2} \text{ regularizer}} + C \sum_{n=1}^{N} [1 - t_{n} y(\mathbf{x}_{n})]_{+}$$

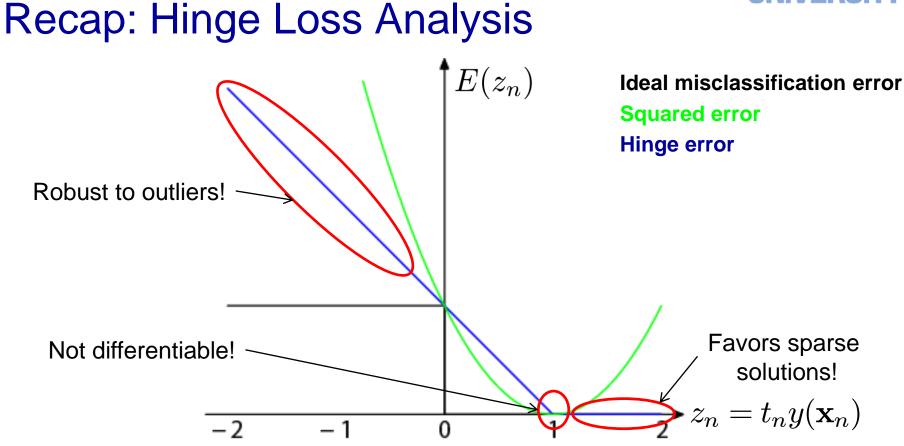
$$\underbrace{\mathbf{L}_{2} \text{ regularizer}}_{\mathbf{H}_{2} \text{ regularizer}} \quad \text{``Hinge loss''}$$

$$\text{where } [x]_{+} := \max\{0, x\}.$$

Slide adapted from Christoph Lampert

Machine Learning Winter '19





- "Hinge error" used in SVMs
 - > Zero error for points outside the margin $(z_n > 1) \implies$ sparsity
 - > Linear penalty for misclassified points ($z_n < 1$) \Rightarrow robustness
 - > Not differentiable around $z_n = 1 \Rightarrow$ Cannot be optimized directly.



Topics of This Lecture

• Recap: Nonlinear Support Vector Machines

- Ensembles of classifiers
 - Bagging
 - Bayesian Model Averaging
- AdaBoost
 - Intuition
 - Algorithm
 - Analysis
 - Extensions

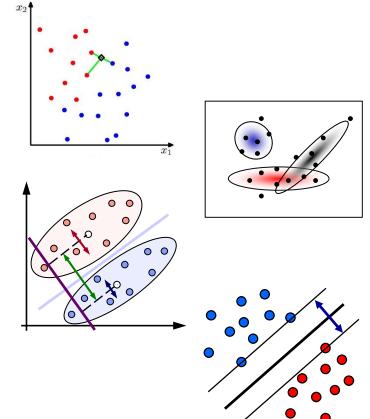


So Far...

- We've seen already a variety of different classifiers
 - ≻ k-NN
 - Bayes classifiers

Linear discriminants

SVMs



- Each of them has their strengths and weaknesses...
 - Can we improve performance by combining them?

Ensembles of Classifiers

- Intuition
 - > Assume we have K classifiers.
 - > They are independent (i.e., their errors are uncorrelated).
 - > Each of them has an error probability p < 0.5 on training data.
 - Why can we assume that p won't be larger than 0.5?
 - Then a simple majority vote of all classifiers should have a lower error than each individual classifier...



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



Constructing Ensembles

- Bagging = "Bootstrap aggregation" (Breiman 1996)
 - > In each run of the training algorithm, randomly select M samples with replacement from the full set of N training data points.
 - > 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 multiple runs of the learning algorithm with different random initializations.

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.
 - > 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.



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



Model Averaging: Expected Error

• Average error of individual models

Average error of committee

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

$$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

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

 $\mathbb{E}_{\mathbf{x}}\left[\epsilon_m(\mathbf{x})\right] = 0$

 $\mathbb{E}_{\mathbf{x}}\left[\epsilon_m(\mathbf{x})\epsilon_j(\mathbf{x})\right] = 0$

- Assumptions
 - > Errors have zero mean:
 - > Errors are uncorrelated:

• Then:

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



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

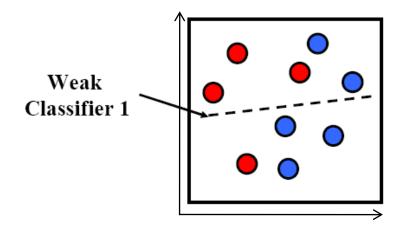
[Freund & Schapire, 1996]

- 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
 - > $H(\mathbf{x})$: "strong" or final classifier
- AdaBoost:
 - Construct a strong classifier as a thresholded linear combination of the weighted weak classifiers:

$$H(\mathbf{x}) = sign\left(\sum_{\substack{m=1\\B \ l \ \text{eibe}}}^{M} \alpha_m h_m(\mathbf{x})\right)$$

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AdaBoost: Intuition

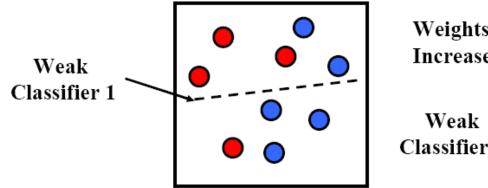


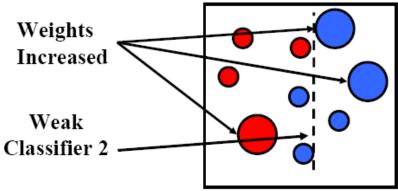
Consider a 2D feature space with positive and negative examples.

Each weak classifier splits the training examples with at least 50% accuracy.

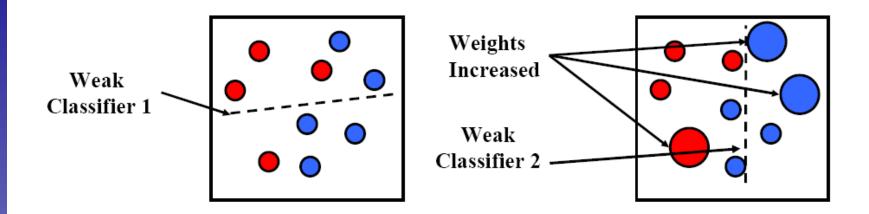
Examples misclassified by a previous weak learner are given more emphasis at future rounds.

AdaBoost: Intuition



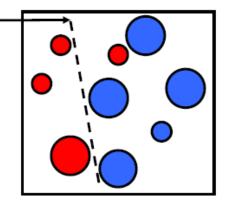


AdaBoost: Intuition



Weak classifier 3

The final classifier is a linear combination of the weak classifiers



Slide credit: Kristen Grauman



AdaBoost – Formalization

- 2-class classification problem
 - > Given: training set $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ with target values $\mathbf{T} = \{t_1, ..., t_N\}, t_n \in \{-1, 1\}$.
 - > Associated weights $\mathbf{W} = \{w_1, ..., w_N\}$ for each training point.
- Basic steps
 - > In each iteration, AdaBoost trains a new weak classifier $h_m(\mathbf{x})$ based on the current weighting coefficients $\mathbf{W}^{(m)}$.
 - > We then adapt the weighting coefficients for each point
 - Increase w_n if \mathbf{x}_n was misclassified by $h_m(\mathbf{x})$.
 - Decrease w_n if \mathbf{x}_n was classified correctly by $h_m(\mathbf{x})$.
 - Make predictions using the final combined model

$$H(\mathbf{x}) = sign\left(\sum_{\substack{m=1\\\text{B. Leibe}}}^{M} \alpha_m h_m(\mathbf{x})\right)$$



AdaBoost – Algorithm

1. Initialization: Set
$$w_n^{(1)} = \frac{1}{N}$$
 for $n = 1, ..., N$.

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.

• Exponential error function

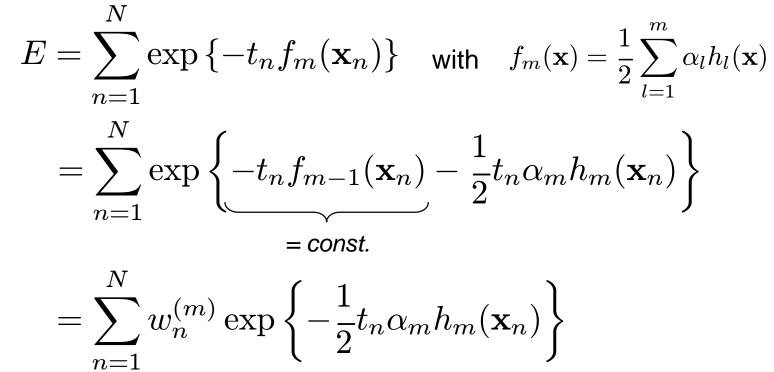
$$E = \sum_{n=1}^{N} \exp\left\{-t_n f_m(\mathbf{x}_n)\right\}$$

> where $f_m(\mathbf{x})$ is a classifier defined as a linear combination of base classifiers $h_l(\mathbf{x})$:

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

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

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



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

- > Observation:
 - Correctly classified points: $t_n h_m(\mathbf{x}_n) = +1 \implies$ collect in \mathcal{T}_m
 - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$

 $\Rightarrow \text{ collect in } \mathcal{T}_m$ $\Rightarrow \text{ collect in } \mathcal{F}_m$

Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$
$$= \left(e^{\alpha_m/2}\right) \sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n)$$

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

- Observation:
 - Correctly classified points: $t_n h_m(\mathbf{x}_n) = +1 \implies \text{collect in } \mathcal{T}_m$
 - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$

$$\Rightarrow$$
 collect in \mathcal{F}_m
 \Rightarrow collect in \mathcal{F}_m

Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$
$$= \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^N w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^N w_n^{(m)}$$

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

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

= const. = 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)

 \Rightarrow We're on the right track. Let's continue...

• Minimize with respect to α_m : $\frac{\partial E}{\partial \alpha_m} \stackrel{!}{=} 0$

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

$$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

- Remaining step: update the weights
 - Recall that

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

This becomes $w_n^{(m+1)}$
in the next iteration

Therefore

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

 \Rightarrow 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

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

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 $h_m(\mathbf{x})$:

$$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

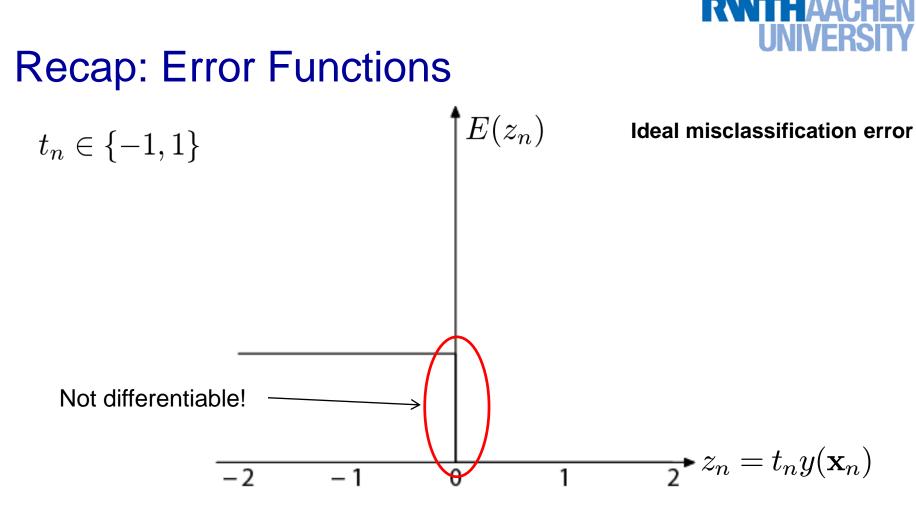
d) Update the weighting coefficients:

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

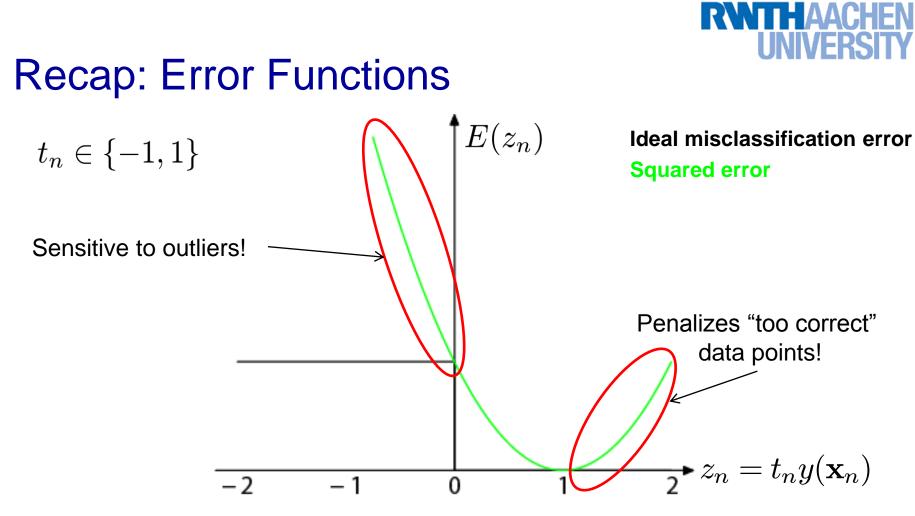


AdaBoost – Analysis

- 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.



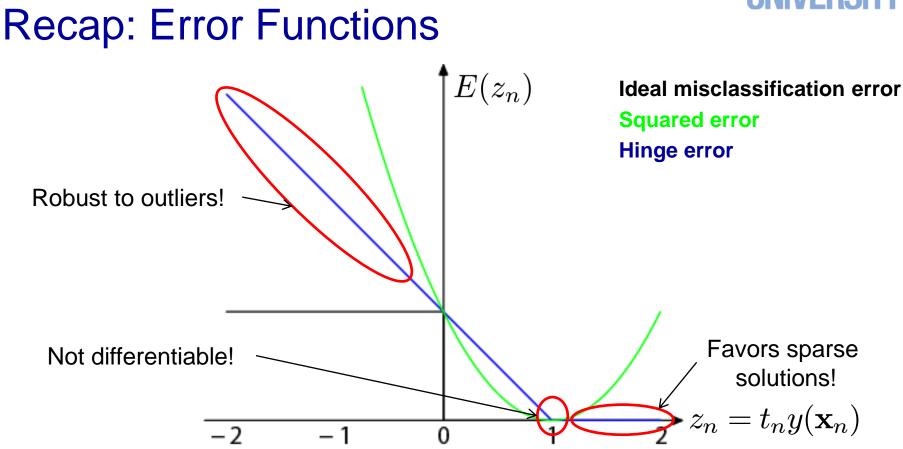
- Ideal misclassification error function (black)
 - > This is what we want to approximate,
 - > Unfortunately, it is not differentiable.
 - > The gradient is zero for misclassified points.
 - \Rightarrow We cannot minimize it by gradient descent.



Squared error used in Least-Squares Classification

- Very popular, leads to closed-form solutions.
- > However, sensitive to outliers due to squared penalty.
- > Penalizes "too correct" data points
- \Rightarrow Generally does not lead to good classifiers.



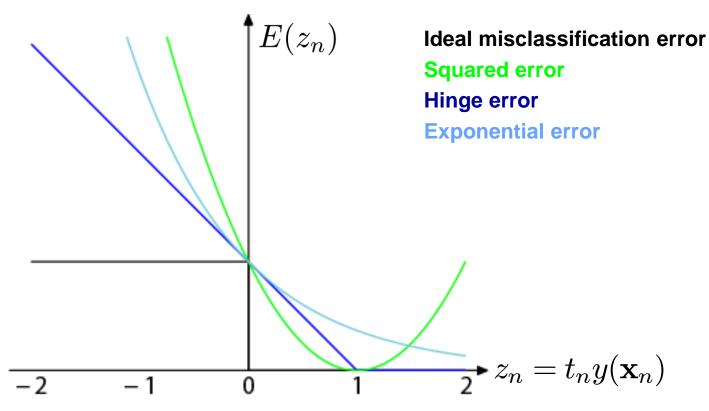


"Hinge error" used in SVMs

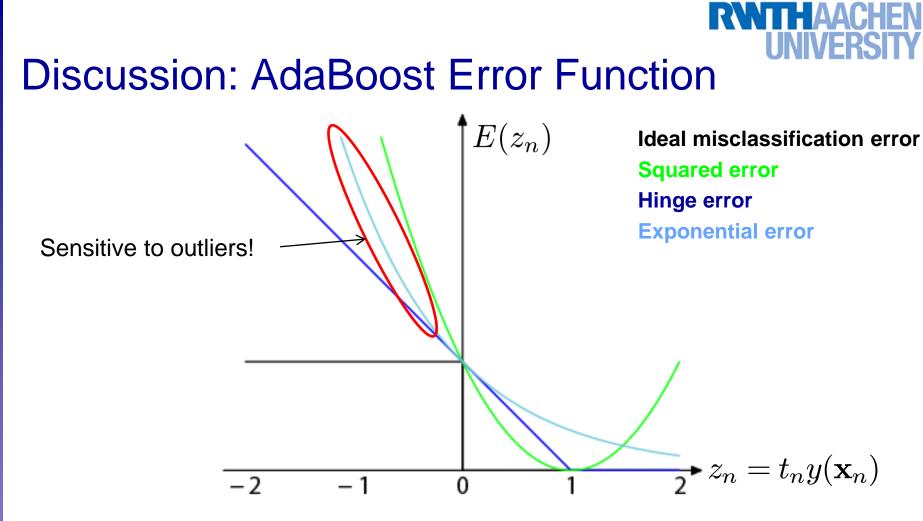
- Zero error for points outside the margin $(z_n > 1) \Rightarrow$ sparsity
- > Linear penalty for misclassified points $(z_n < 1) \implies$ robustness
- > Not differentiable around $z_n = 1 \Rightarrow$ Cannot be optimized directly.

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Discussion: AdaBoost Error Function

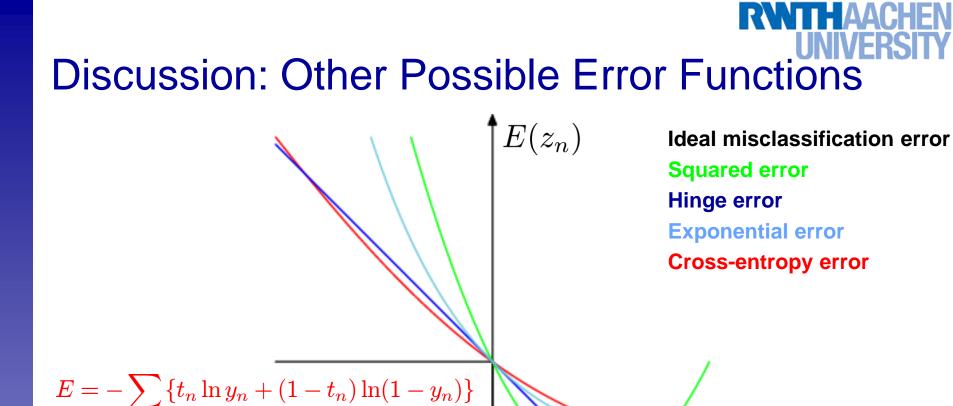


- Exponential error used in AdaBoost
 - Continuous approximation to ideal misclassification function.
 - Sequential minimization leads to simple AdaBoost scheme.
 - > Properties?



Exponential error used in AdaBoost

- No penalty for too correct data points, fast convergence.
- > Disadvantage: exponential penalty for large negative values!
- \Rightarrow Less robust to outliers or misclassified data points!



- "Cross-entropy error" used in Logistic Regression
 - > Similar to exponential error for z>0.

-2

- > Only grows linearly with large negative values of z.
- \Rightarrow Make AdaBoost more robust by switching to this error function.

0

 \Rightarrow "GentleBoost"

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 $\rightarrow z_n = t_n y(\mathbf{x}_n)$

Summary: AdaBoost

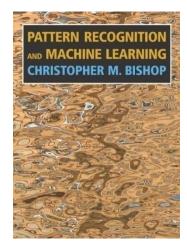
- Properties
 - Simple combination of multiple classifiers.
 - Easy to implement.
 - Can be used with many different types of classifiers.
 - None of them needs to be too good on its own.
 - In fact, they only have to be slightly better than chance.
 - Commonly used in many areas.
 - Empirically good generalization capabilities.
 - Limitations
 - Original AdaBoost sensitive to misclassified training data points.
 - Because of exponential error function.
 - Improvement by GentleBoost
 - Single-class classifier
 - Multiclass extensions available



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</u> <u>Statistical View of Boosting</u>, *The Annals of Statistics*, Vol. 38(2), pages 337-374, 2000.