Machine Learning – Lecture 9

Model Combination

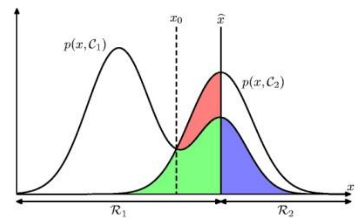
13.11.2017

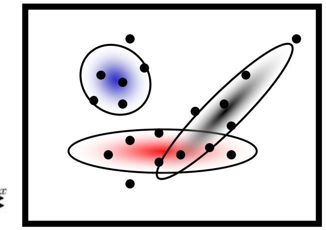
Bastian Leibe
RWTH Aachen
http://www.vision.rwth-aachen.de

leibe@vision.rwth-aachen.de

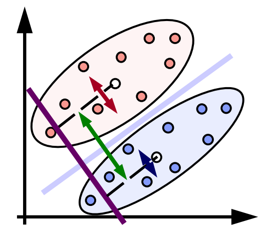
Course Outline

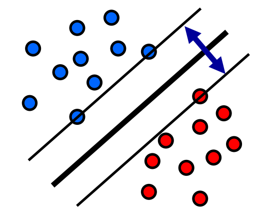
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation

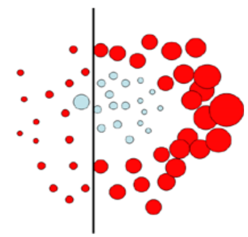


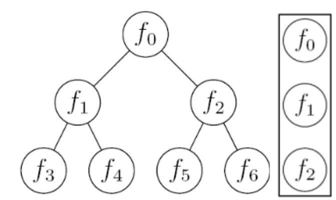


- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns

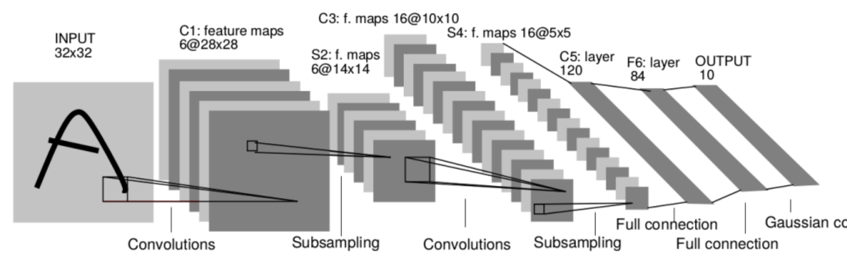








- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

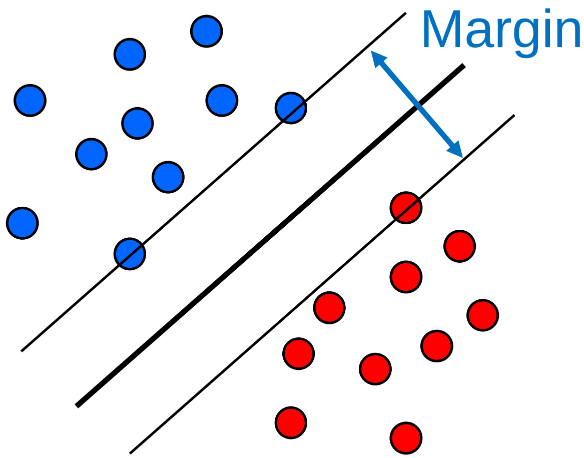


Topics of This Lecture

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

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

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

under the constraints

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

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

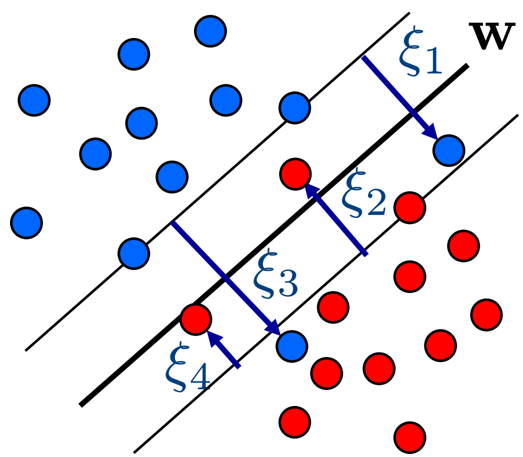
$$a_n \geq 0 \quad \forall n$$

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

- Comparison
  - 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 $\mathcal{O}(N^2)$.

Recap: SVM for Non-Separable Data

- Slack variables
  - One slack variable $\xi_n \geq 0$ 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: $\xi_n = 1$

Misclassified point: $\xi_n > 1$

  - We do not have to set the slack variables ourselves!

$\Rightarrow$ They are jointly optimized together with $\mathbf{w}$.

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

$$0 \cdot \quad a_n \cdot \quad C$$

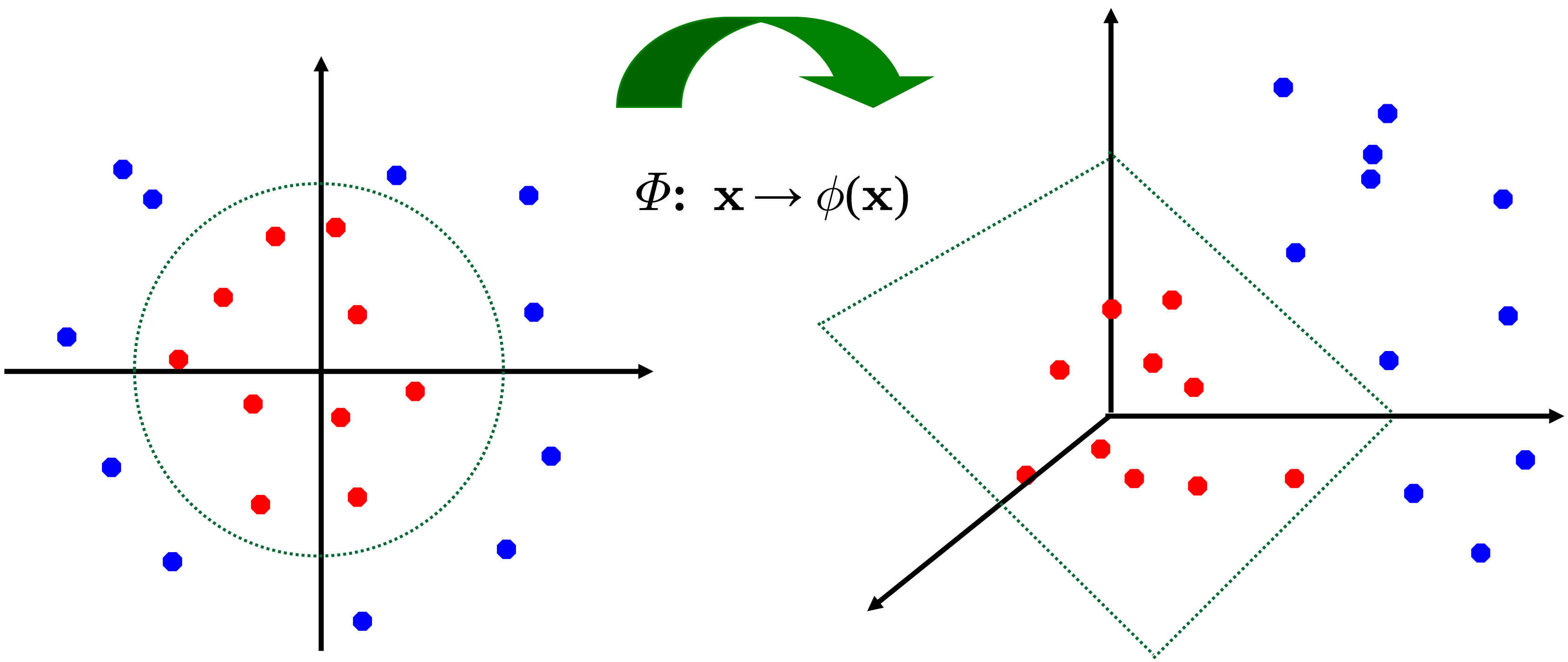
$$\sum_{n=1}^{N} a_n t_n \; = \; 0$$

This is all that changed!

- This is again a quadratic programming problem
  - $\Rightarrow$ Solve as before…

Recap: Nonlinear SVMs

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



Slide credit: Raymond Mooney

Recap: The Kernel Trick

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

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

  - 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 higher-dimensional space (without having to compute $\phi(\mathbf{x})$ explicitly)!

Nonlinear SVM – Dual Formulation

- SVM Dual: Maximize

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

under the conditions

$$0 \cdot \quad a_n \cdot \quad C$$

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

- Classify new data points using

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

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-machines.org/

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 $y(\mathbf{x})$ scales linearly in the number of SVs.
    - Too expensive if we have a large number of support vectors.

    $\Rightarrow$ 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

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

SVM – Analysis

- Traditional soft-margin formulation

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

"Maximize the margin"

subject to the constraints

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

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

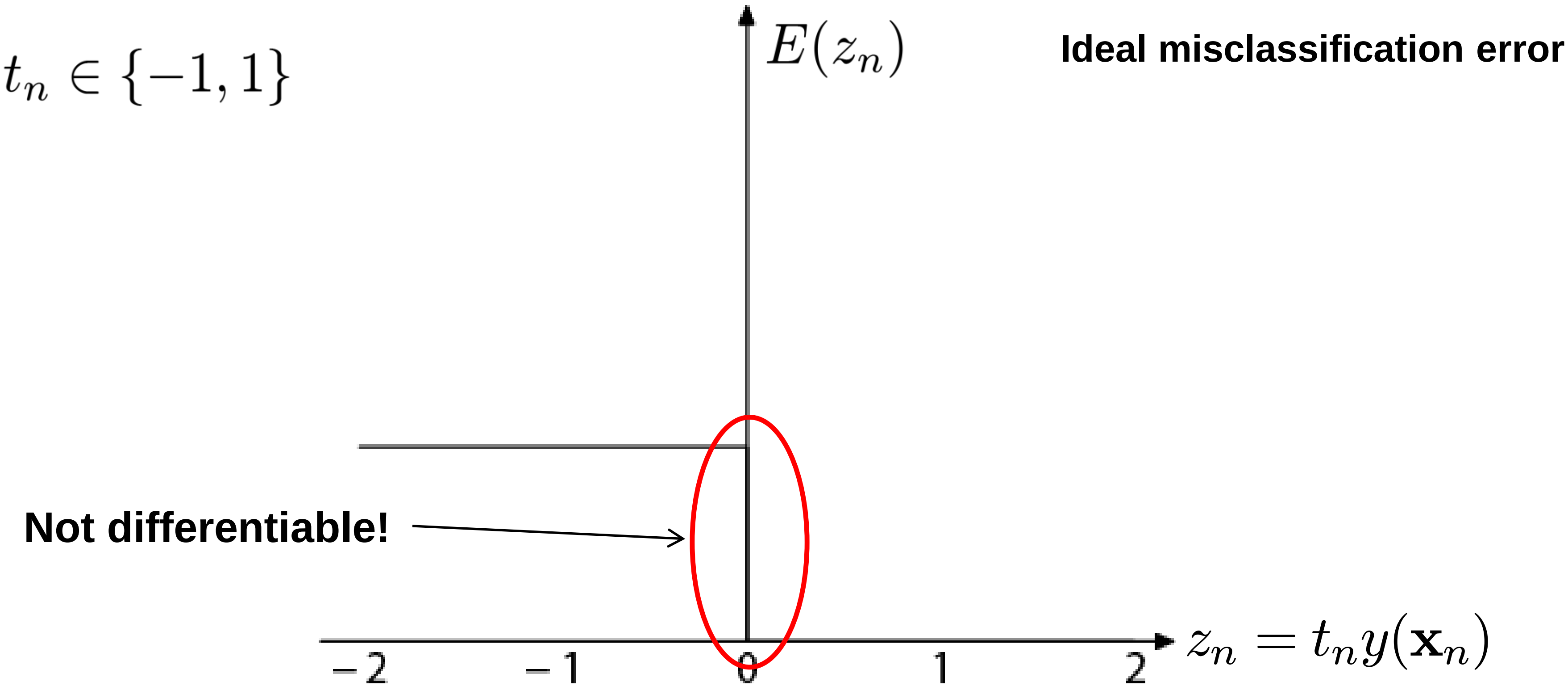
- Different way of looking at it
  - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{L_2 \text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{"Hinge loss"}}$$

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

Recap: Error Functions

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

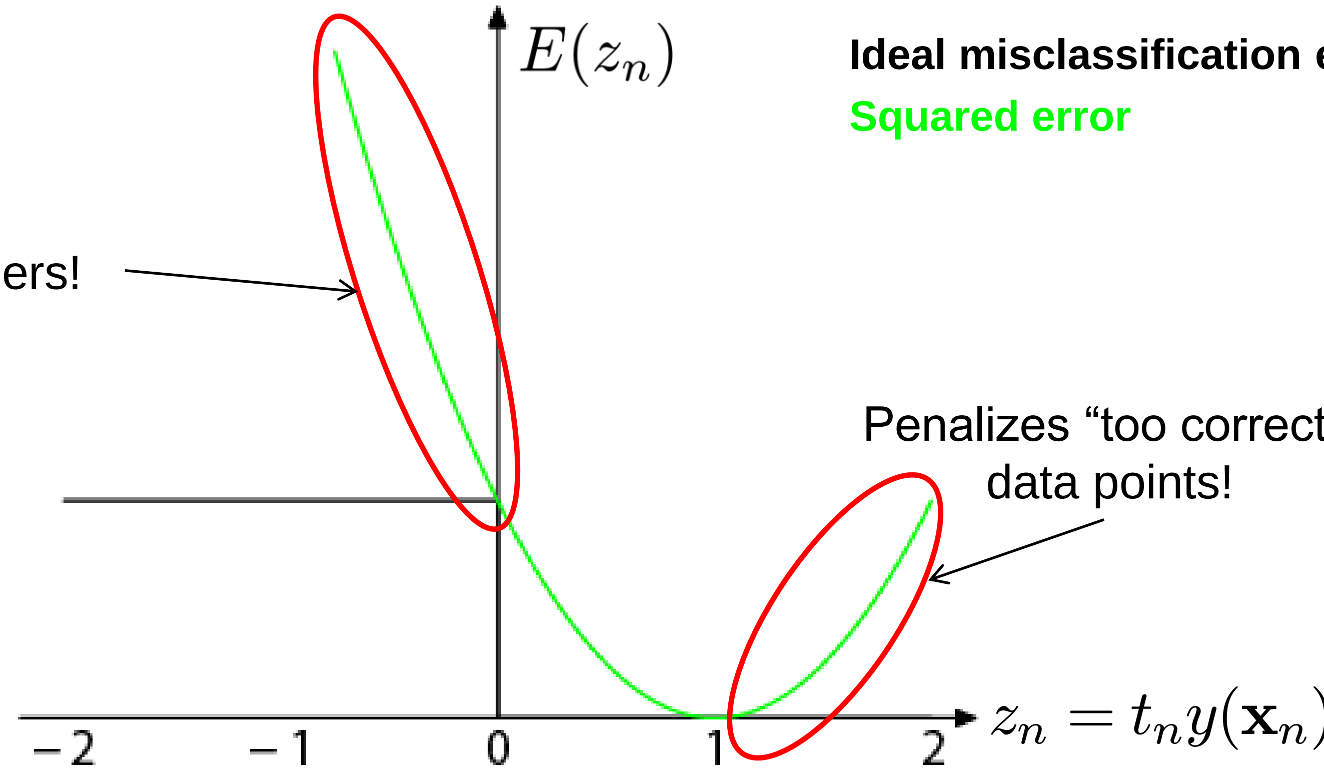


- Ideal misclassification error function (black)
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.
  - $\Rightarrow$ We cannot minimize it by gradient descent.

Image source: Bishop, 2006

Recap: Error Functions

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

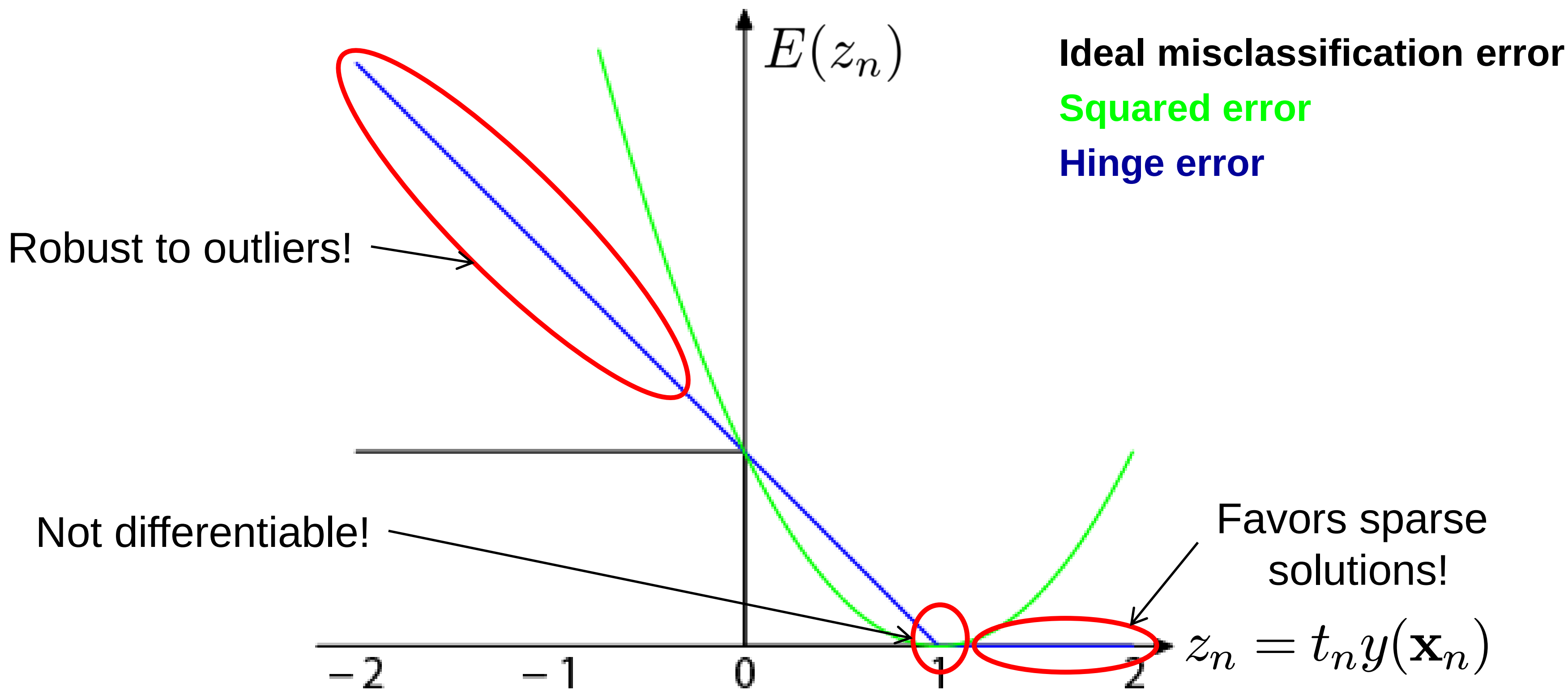


- Squared error used in Least-Squares Classification
  - Very popular, leads to closed-form solutions.
  - However, sensitive to outliers due to squared penalty.
  - Penalizes "too correct" data points

  $\Rightarrow$ Generally does not lead to good classifiers.

Image source: Bishop, 2006

Error Functions (Loss Functions)



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

Image source: Bishop, 2006

SVM – Discussion

- SVM optimization function

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{L_2 \text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1-t_n y(\mathbf{x}_n)]_+}_{\text{Hinge loss}}$$

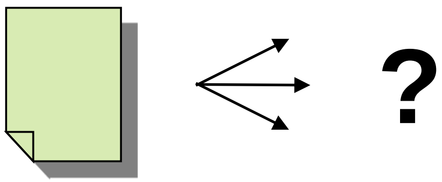
- Hinge loss enforces sparsity
  - Only a subset of training data points actually influences the decision boundary.
  - This is different from sparsity obtained through the regularizer! There, only a subset of input dimensions are used.
  - Unconstrained optimization, but non-differentiable function.
  - Solve, e.g. by *subgradient descent*
  - Currently most efficient: *stochastic gradient descent*

Topics of This Lecture

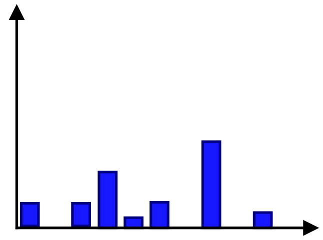
- Recap: Nonlinear Support Vector Machines
- Analysis
  - Error function
- Applications
- Ensembles of classifiers
  - Bagging
  - Bayesian Model Averaging
- AdaBoost
  - Intuition
  - Algorithm
  - Analysis
  - Extensions

Example Application: Text Classification

- Problem:
  - Classify a document in a number of categories



- Representation:
  - "Bag-of-words" approach
  - Histogram of word counts (on learned dictionary)
    - Very high-dimensional feature space (~10.000 dimensions)
    - Few irrelevant features



- This was one of the first applications of SVMs
  - T. Joachims (1997)

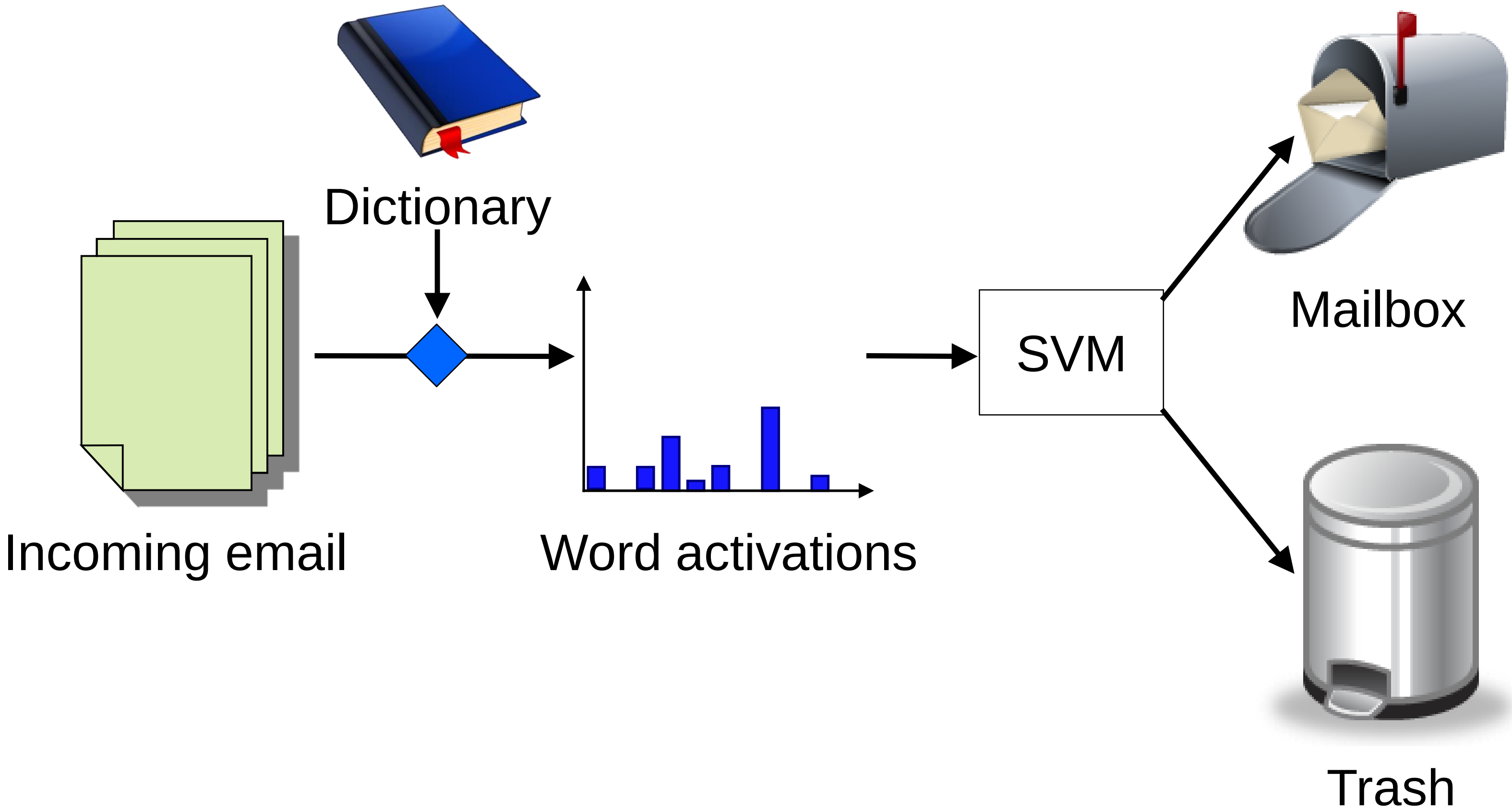
Example Application: Text Classification

- Results:

	Bayes	Rocchio	C4.5	k-NN	SVM (poly) degree $d=$ 1	2	3	4	5	SVM (rbf) width $\gamma=$ 0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	**98.5**	98.4	98.3	**98.5**	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	**95.2**	95.2	95.3	95.0	95.3	95.3	**95.4**
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	**76.2**	74.0	75.4	**76.3**	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	**92.4**	91.3	89.9	**93.1**	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	**88.9**	87.8	**88.9**	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	**77.1**	76.9	78.0	**77.8**	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	**76.2**	74.4	75.0	**76.2**	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	**86.5**	86.0	**85.4**	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	**85.9**	83.8	**85.2**	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	**85.7**	83.9	**85.1**	85.7	85.7	84.5
microavg.	**72.0**	**79.9**	**79.4**	**82.3**	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2
					combined: **86.0**					combined: **86.4**			

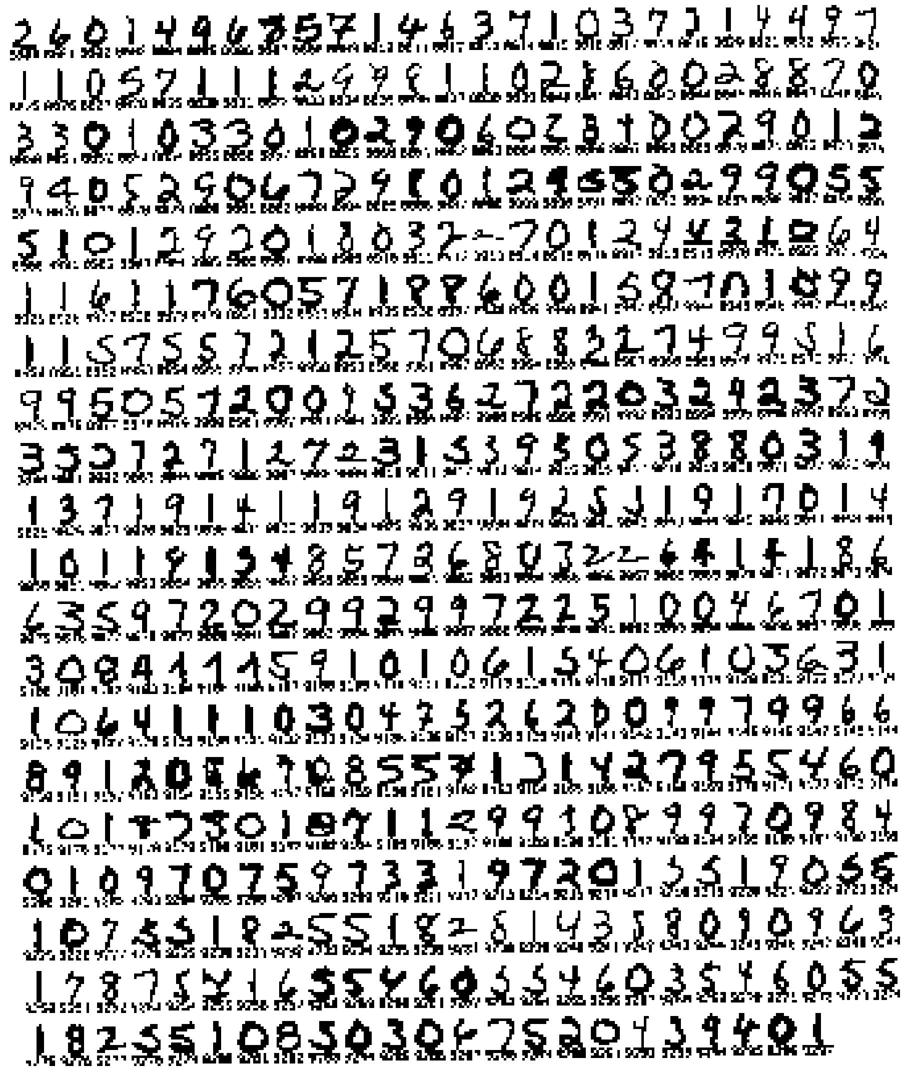
Example Application: Text Classification

- This is also how you could implement a simple spam filter…



Example Application: OCR

- Handwritten digit recognition
  - US Postal Service Database
  - Standard benchmark task for many learning algorithms



Historical Importance

- USPS benchmark
  - 2.5% error: human performance
- Different learning algorithms
  - 16.2% error: Decision tree (C4.5)
  - 5.9% error: (best) 2-layer Neural Network
  - 5.1% error: LeNet 1 – (massively hand-tuned) 5-layer network
- Different SVMs
  - 4.0% error: Polynomial kernel (p=3, 274 support vectors)
  - 4.1% error: Gaussian kernel (σ=0.3, 291 support vectors)

Example Application: OCR

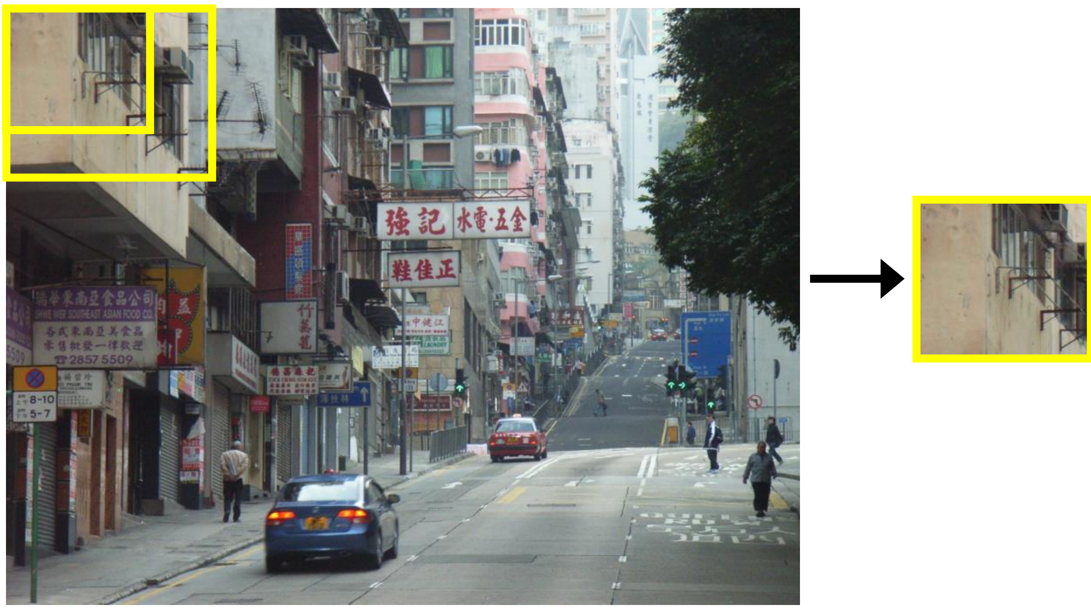
- Results
  - Almost no overfitting with higher-degree kernels.

degree of polynomial	dimensionality of feature space	support vectors	raw error
1	256	282	8.9
2	≈ 33000	227	4.7
3	$\approx 1 \times 10^6$	274	4.0
4	$\approx 1 \times 10^9$	321	4.2
5	$\approx 1 \times 10^{12}$	374	4.3
6	$\approx 1 \times 10^{14}$	377	4.5
7	$\approx 1 \times 10^{16}$	422	4.5

Example Application: Object Detection

Real-time capable!

- Sliding-window approach



Obj./non-obj. Classifier

- E.g. histogram representation (HOG)
  - Map each grid cell in the input window to a histogram of gradient orientations.
  - Train a linear SVM using training set of pedestrian vs. non-pedestrian windows.

[Dalal & Triggs, CVPR 2005]

Example Application: Pedestrian Detection

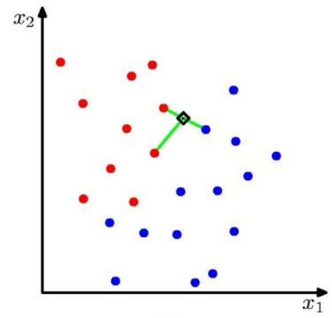
N. Dalal, B. Triggs, Histograms of Oriented Gradients for Human Detection, CVPR 2005

Topics of This Lecture

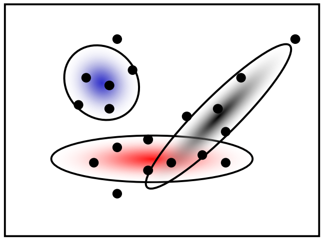
- Recap: Nonlinear Support Vector Machines
- Analysis
  - Error function
- Applications
- Ensembles of classifiers
  - Bagging
  - Bayesian Model Averaging
- AdaBoost
  - Intuition
  - Algorithm
  - Analysis
  - Extensions

So Far…

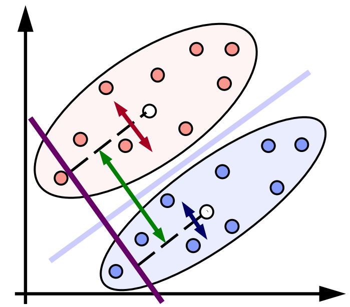
- We've seen already a variety of different classifiers
  - k-NN



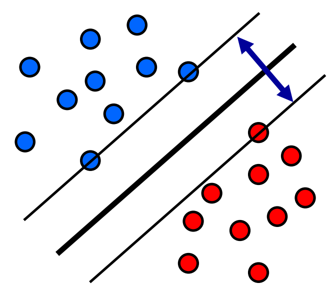
  - Bayes classifiers



  - 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 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 mutliple runs of the learning algorithm with different random initializations.

Bayesian Model Averaging

- Model Averaging
  - Suppose we have H different models $h = 1,\ldots,H$ 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:

$$p(\mathbf{X}) = \sum_{\mathbf{z}} p(\mathbf{X}, \mathbf{z})$$

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

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

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

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

- Assumptions
  - Errors have zero mean: $\mathbb{E}_{\mathbf{x}}\left[\epsilon_m(\mathbf{x})\right] = 0$
  - Errors are uncorrelated: $\mathbb{E}_{\mathbf{x}}\left[\epsilon_m(\mathbf{x})\epsilon_j(\mathbf{x})\right] = 0$

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

Isn't this spectacular?

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

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

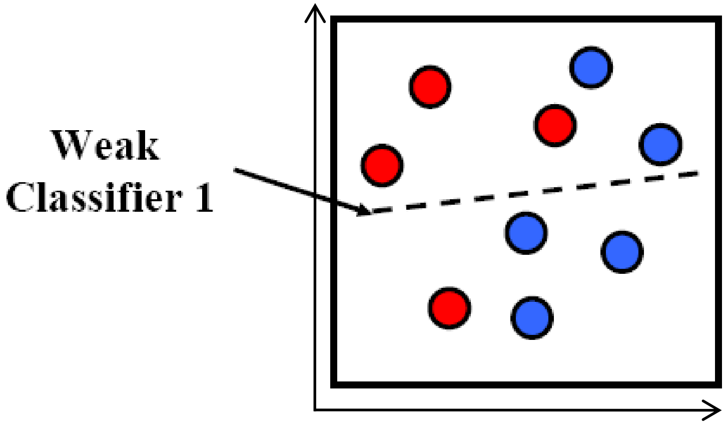
RWTH AACHEN UNIVERSITY

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:

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

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.

Figure adapted from Freund & Schapire

AdaBoost: Intuition

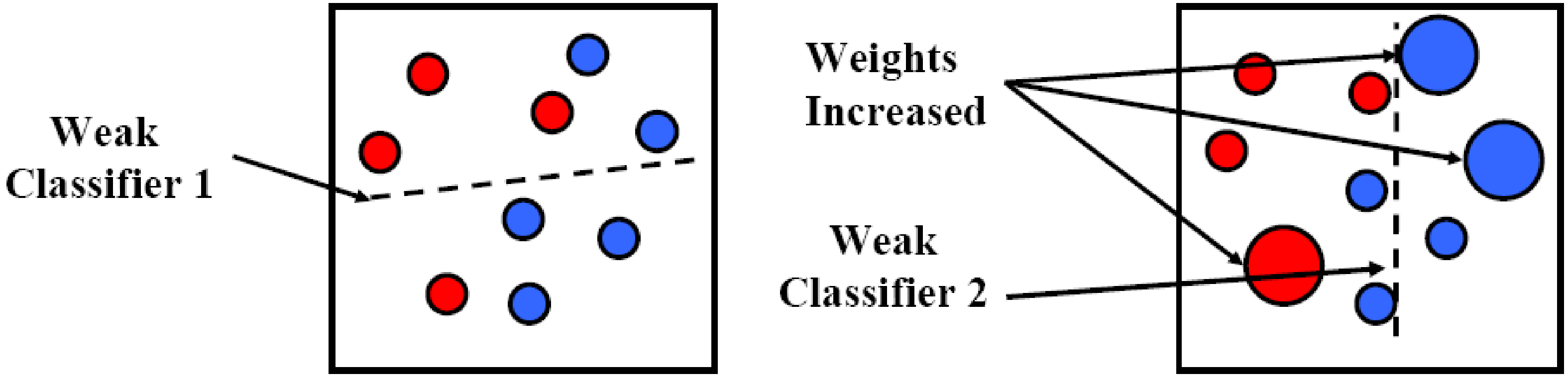
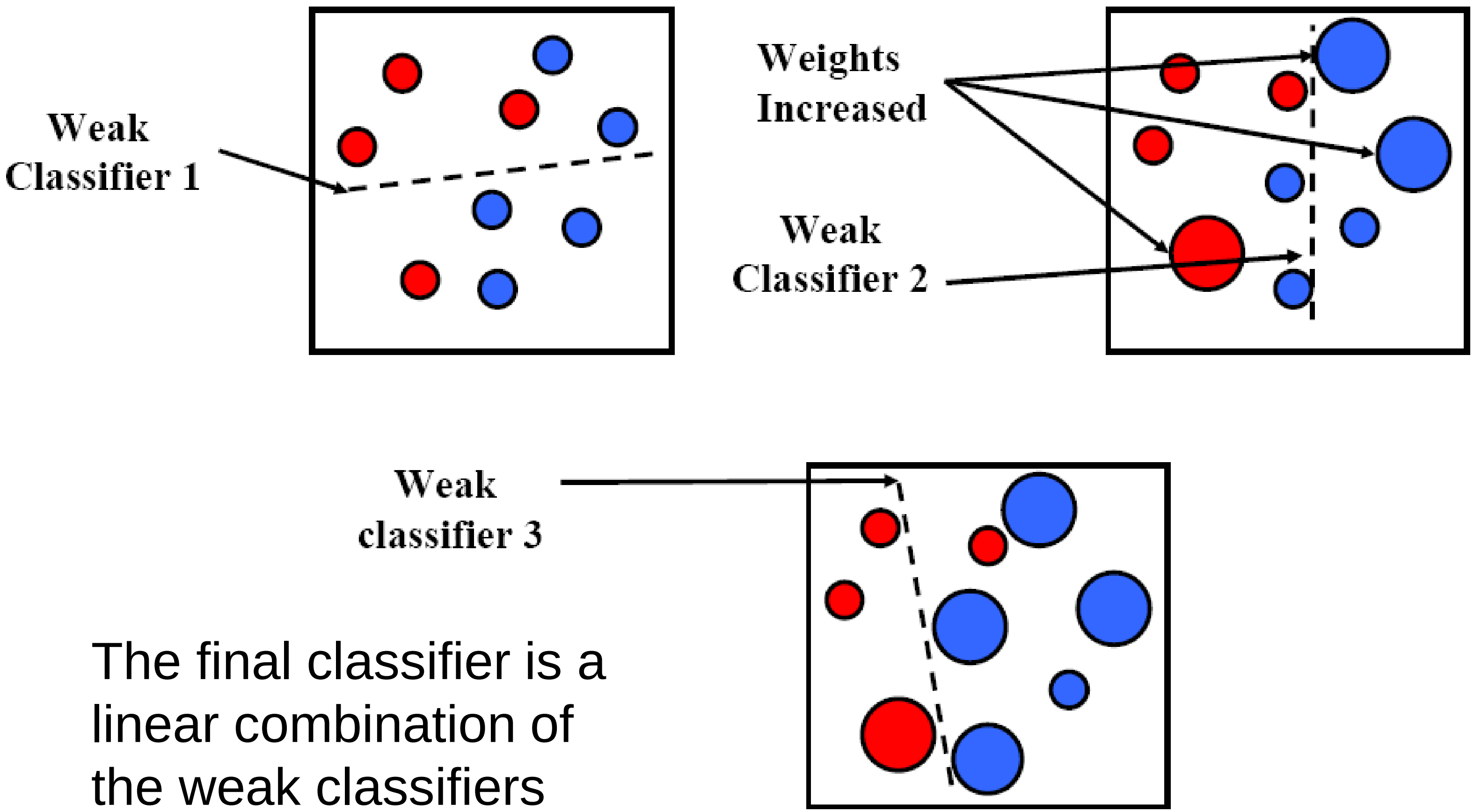


Figure adapted from Freund & Schapire

AdaBoost: Intuition



The final classifier is a linear combination of the weak classifiers

Figure adapted from Freund & Schapire

AdaBoost – Formalization

- 2-class classification problem
  - Given: training set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ with target values $\mathbf{T} = \{t_1, \ldots, t_N\}$, $t_n \in \{-1,1\}$.
  - Associated weights $\mathbf{W}=\{w_1, \ldots, w_N\}$ 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

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

AdaBoost – Algorithm

1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\ldots,N$.
2. For $m = 1,\ldots,M$ 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

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

$$I(A) = \begin{cases} 1, & \text{if } A \text{ is true} \\ 0, & \text{else} \end{cases}$$

   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.

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 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 $h_l(\mathbf{x})$.

AdaBoost – Minimizing Exponential Error

- 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 $h_m(\mathbf{x})$.

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

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

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

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 $\mathcal{T}_m$
  - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$ $\Rightarrow$ collect in $\mathcal{F}_m$
- Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$

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

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 $\mathcal{T}_m$
  - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$ $\Rightarrow$ collect in $\mathcal{F}_m$
- Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$

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

AdaBoost – Minimizing Exponential Error

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

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

$\Rightarrow$ 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…*

AdaBoost – Minimizing Exponential Error

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

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

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

weighted error

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

$$\epsilon_m = \frac{1}{e^{\alpha_m} + 1}$$

$\Rightarrow$ *Update for the α coefficients:*

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

AdaBoost – Minimizing Exponential Error

- Remaining step: update the weights
  - Recall that

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

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

  - Therefore

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

$$= \ldots$$

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

$\Rightarrow$ *Update for the weight coefficients.*

AdaBoost – Final Algorithm

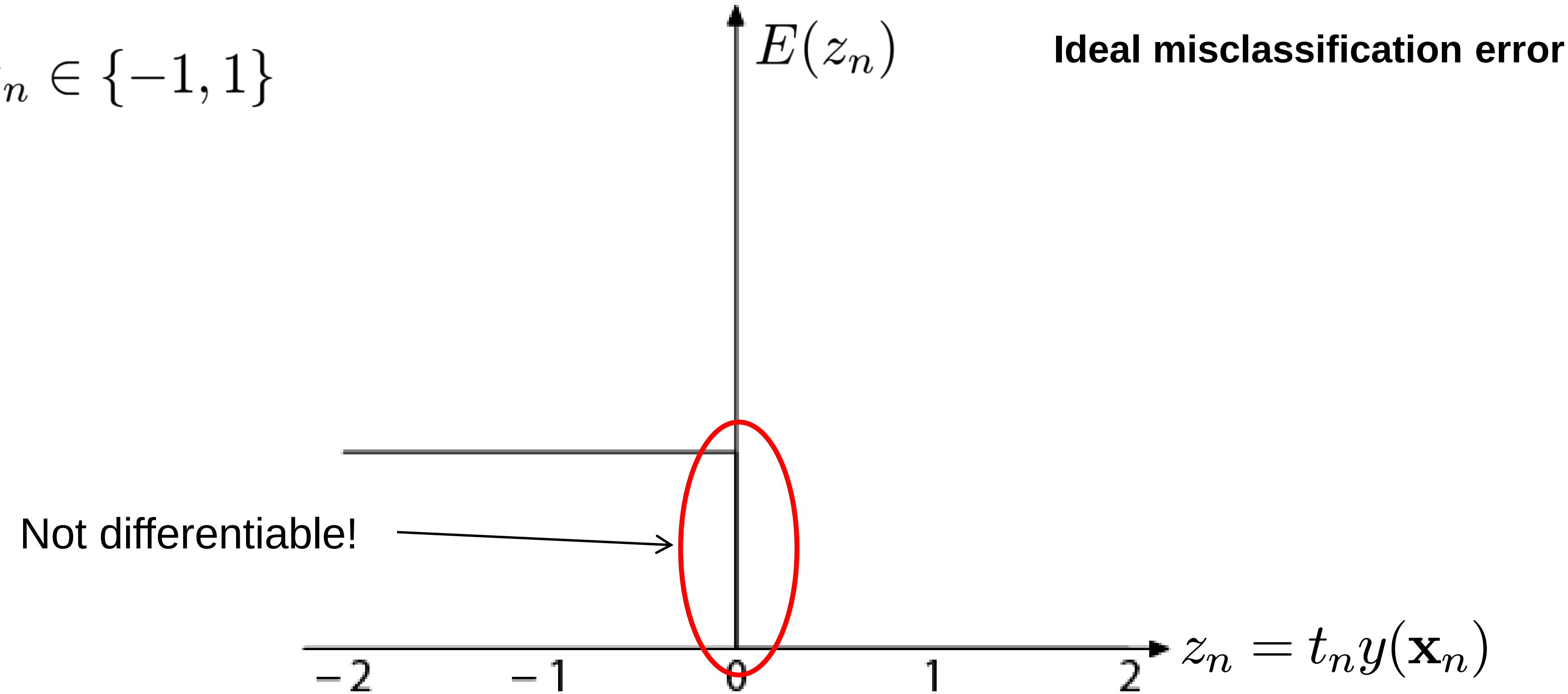
1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\ldots,N$.
2. For $m = 1,\ldots,M$ iterations
   a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function
   $$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x})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

Recap: Error Functions

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



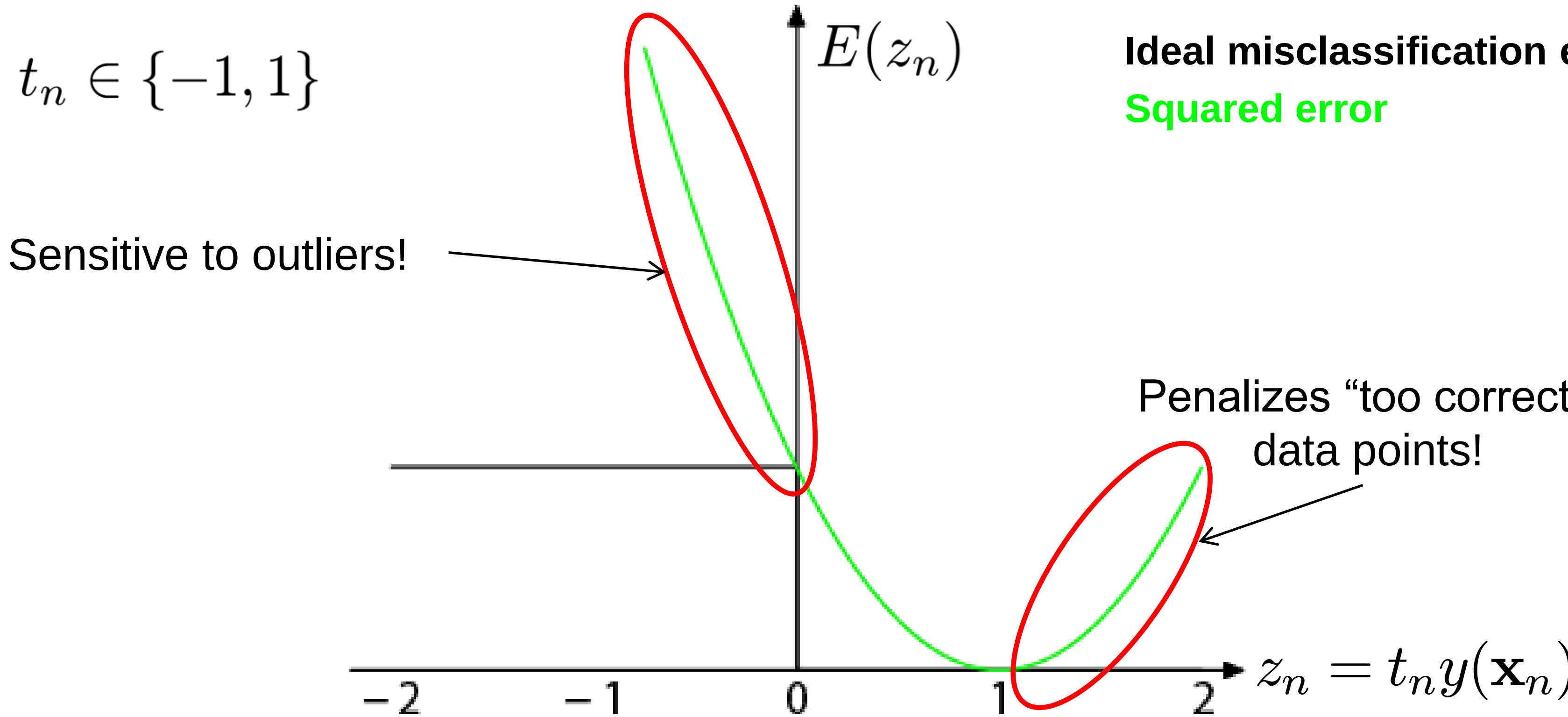
- Ideal misclassification error function (black)
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.

  $\Rightarrow$ We cannot minimize it by gradient descent.

Image source: Bishop, 2006

Recap: Error Functions

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



Ideal misclassification error

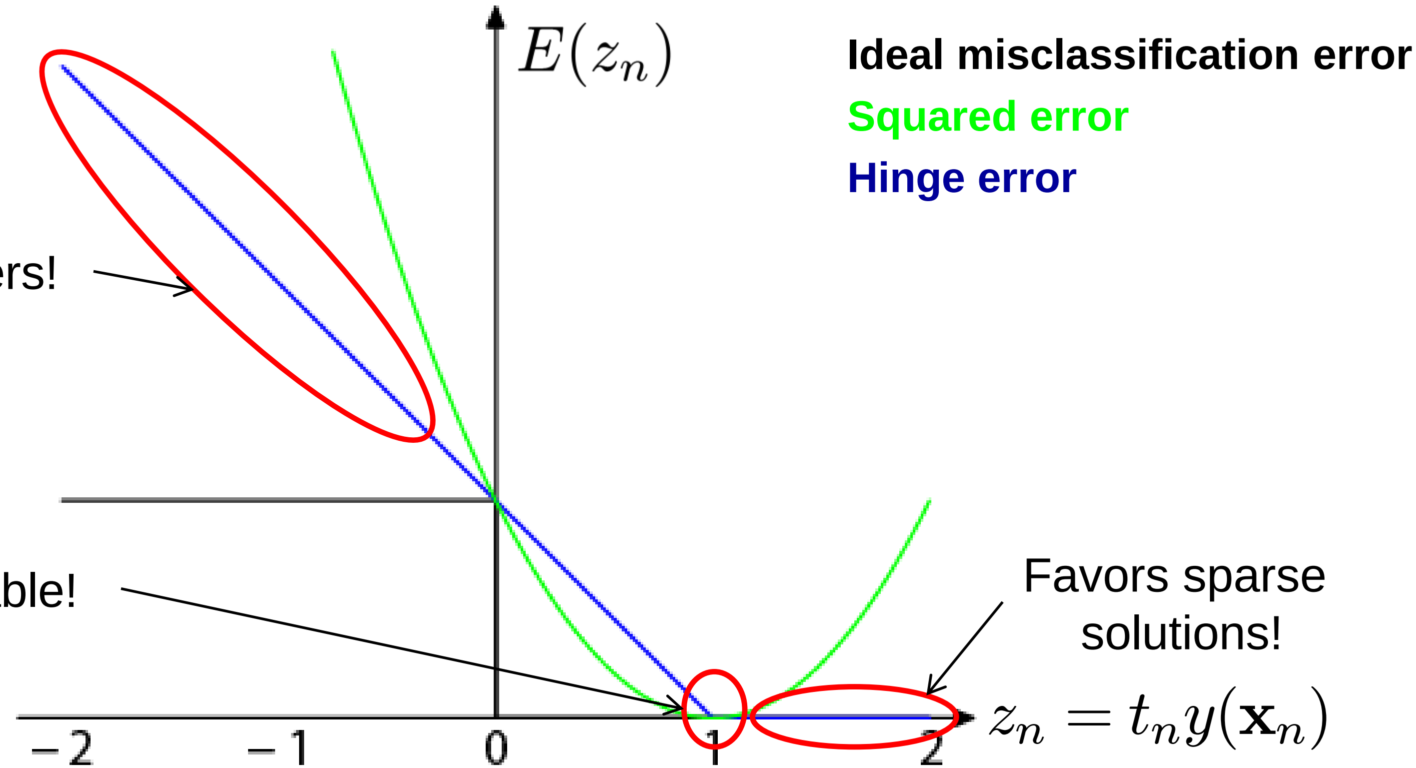
Squared error

- 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

  ⇒ Generally does not lead to good classifiers.

Image source: Bishop, 2006

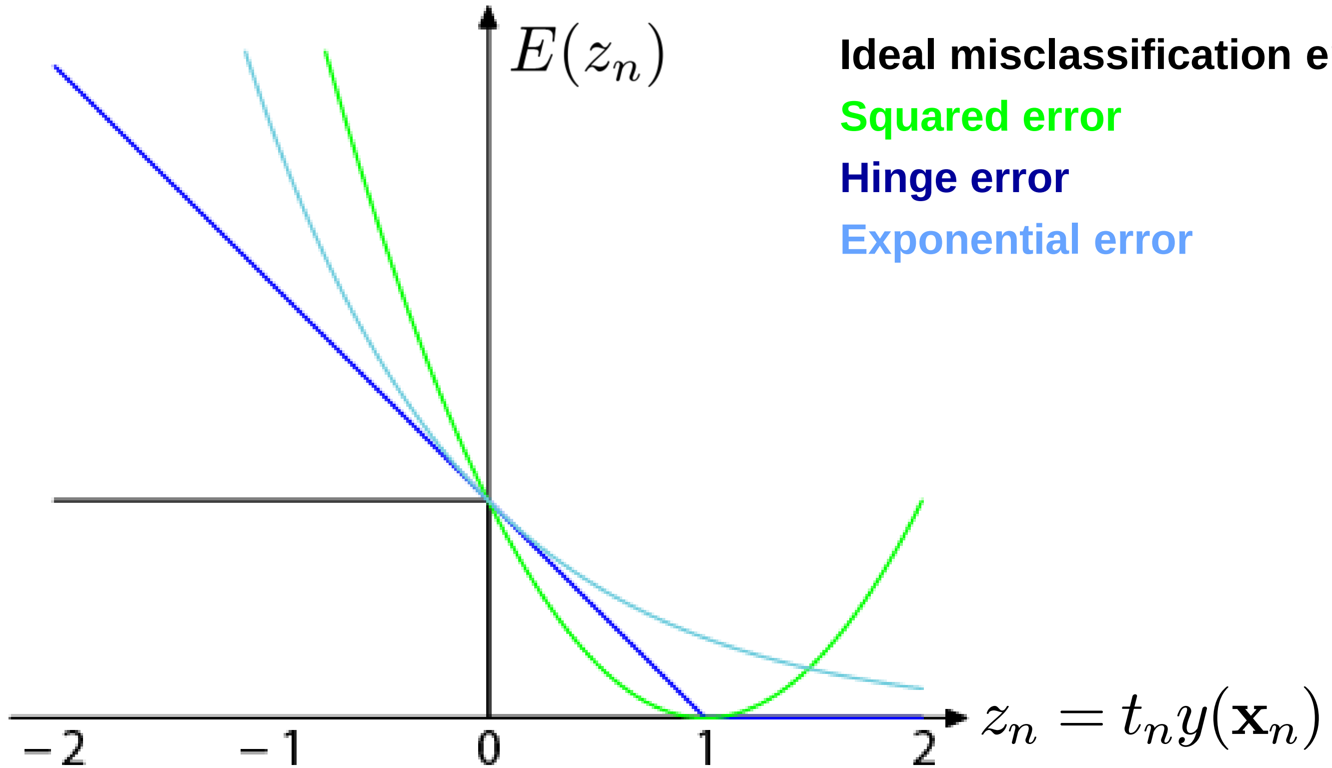
Recap: Error Functions



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

Image source: Bishop, 2006

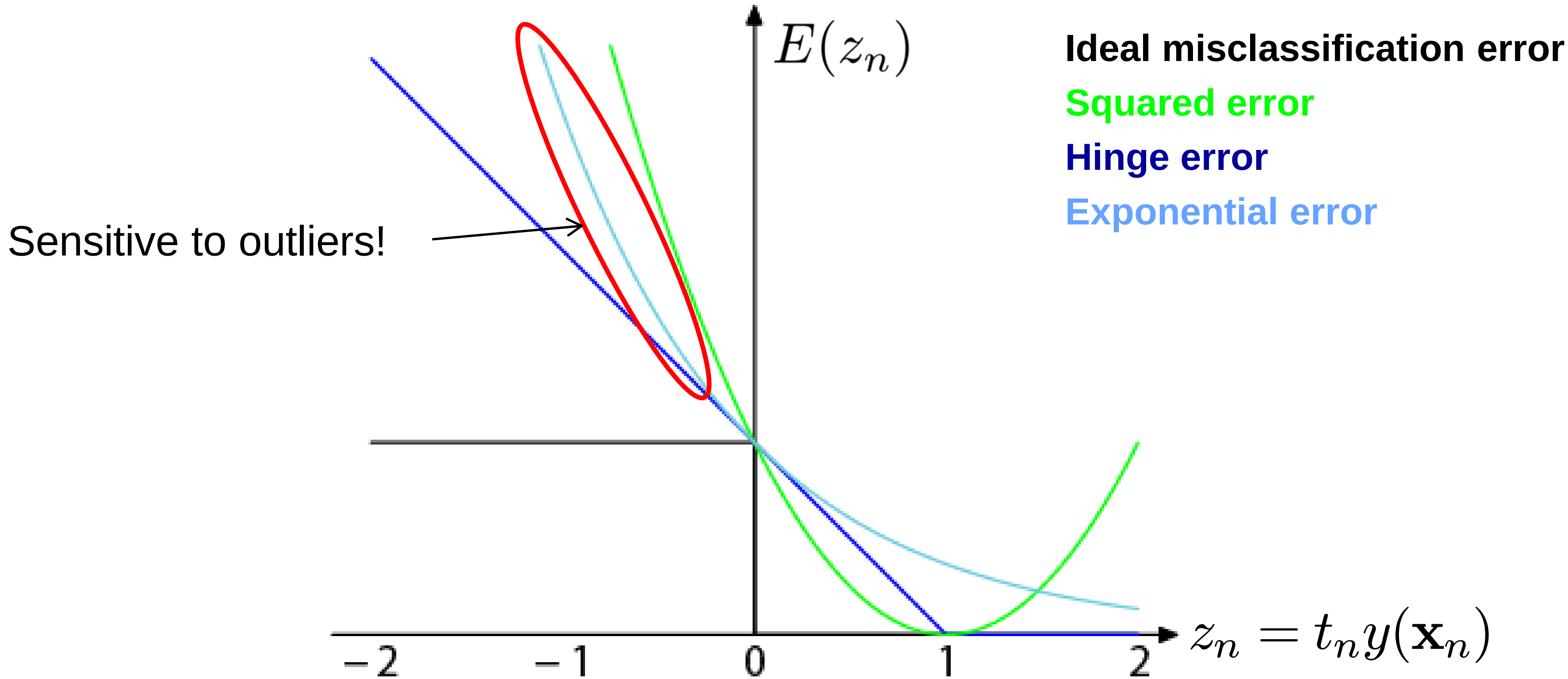
Discussion: AdaBoost Error Function



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

Image source: Bishop, 2006

Discussion: AdaBoost Error Function

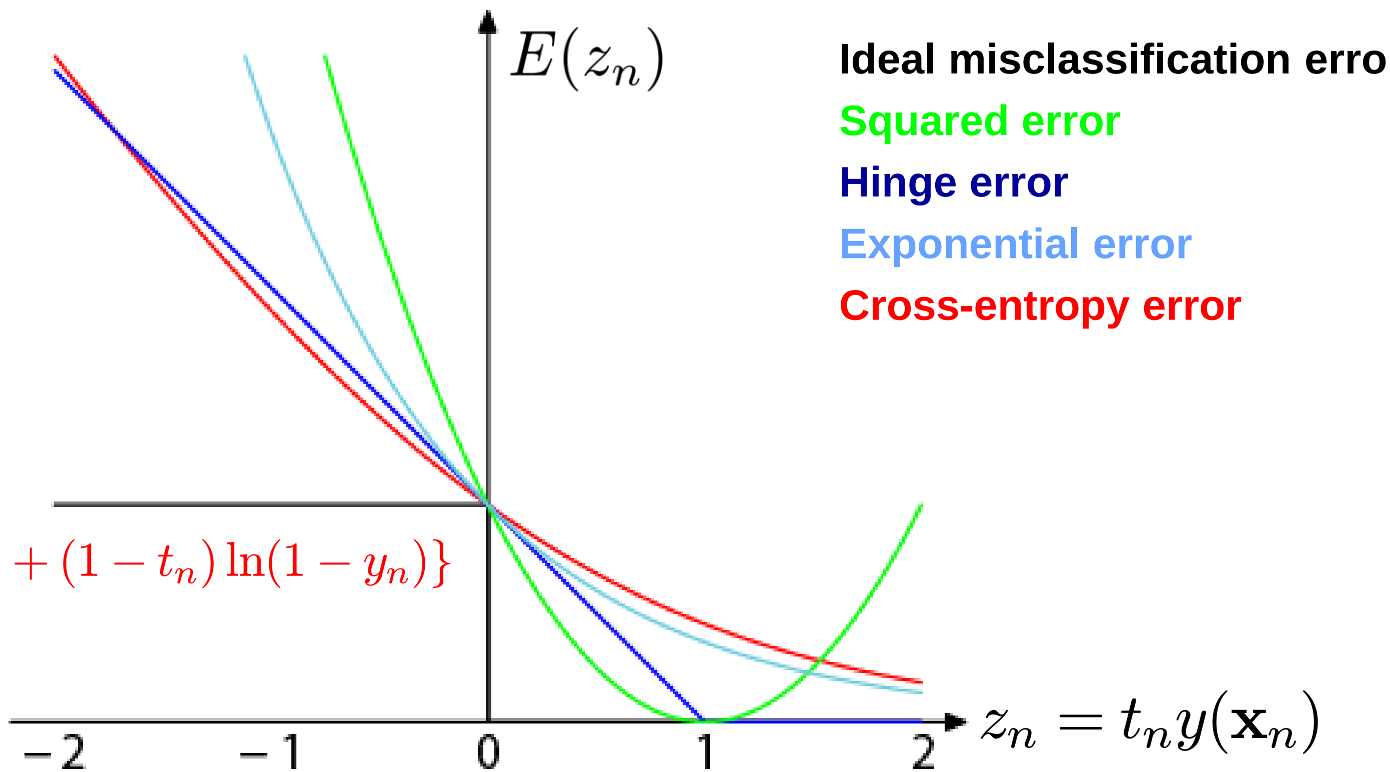


- Exponential error used in AdaBoost
  - No penalty for too correct data points, fast convergence.
  - Disadvantage: exponential penalty for large negative values!

  $\Rightarrow$ Less robust to outliers or misclassified data points!

Image source: Bishop, 2006

Discussion: Other Possible Error Functions



$$E = -\sum \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- "Cross-entropy error" used in Logistic Regression
  - Similar to exponential error for $z>0$.
  - Only grows linearly with large negative values of z.

  $\Rightarrow$ Make AdaBoost more robust by switching to this error function.

  $\Rightarrow$ "GentleBoost"

Image source: Bishop, 2006

Summary: AdaBoost

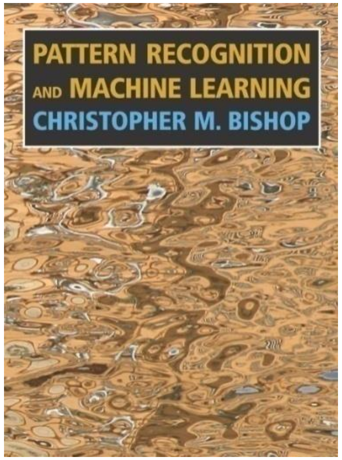
- Properties
  - Simple combination of multiple classifiers.
  - Easy to implement.
  - Can be used with many different types of classifiers.
    - None of them needs to be too good on its own.
    - In fact, they only have to be slightly better than chance.
  - Commonly used in many areas.
  - Empirically 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, Additive Logistic Regression: a Statistical View of Boosting, *The Annals of Statistics*, Vol. 38(2), pages 337-374, 2000.