Machine Learning - Lecture 10

AdaBoost

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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

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 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

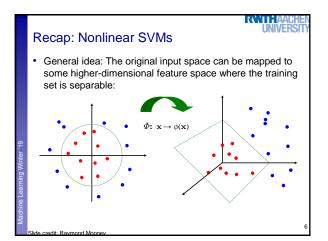
$$L_d(\mathbf{a}) = \sum_{n=1}^N a_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N a_n a_m t_n t_m(\mathbf{x}_m^{\mathrm{T}} \mathbf{x}_n)$$

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under the conditions

$$a_n \ge 0 \quad \forall a \in \sum_{n=1}^{N} a_n t_n = 0$$

- Comparison
 - > L_d is equivalent to the primal form L_p , but only depends on a_n .
 - L_n 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: 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

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

under the conditions

$$0 \cdot a_n \cdot C$$

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

· Classify new data points using

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

Recap: SVM Loss Function

· Traditional soft-margin formulation

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

subject to the constraints

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

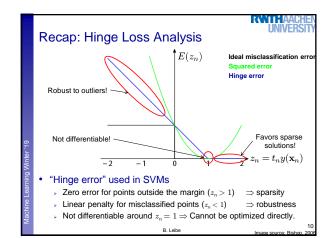
"Most points should be on the correct side of the margin

- Different way of looking at it

We can reformulate the constraints into the objective function.
$$\min_{\mathbf{w} \in \mathbb{R}^D} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N [1 - t_n y(\mathbf{x}_n)]_+$$

$$\mathbf{L}_2 \text{ regularizer} \qquad \text{"Hinge loss"}$$

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



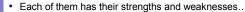
Topics of This Lecture

- 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



> Can we improve performance by combining them?



Ensembles of Classifiers

- Intuition
 - \succ Assume we have K classifiers.
 - > They are independent (i.e., their errors are uncorrelated).
 - \rightarrow 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,...

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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.
 - ightarrow 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,...,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.

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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.
 - \Rightarrow One latent variable ${\bf z}$ 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(x) for target output h(x).
 - E.g. each trained on a different bootstrap data set by bagging.
 - > The committee prediction is given by

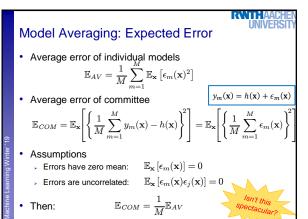
$$y_{COM}(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x})$$

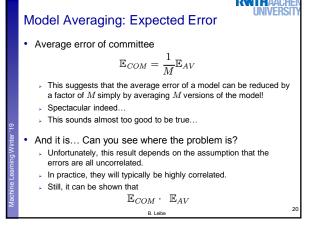
> The output can be written as the true value plus some error.

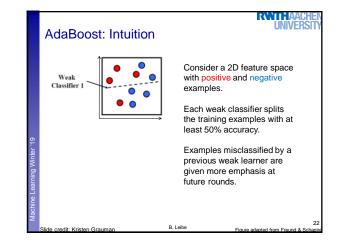
$$y(\mathbf{x}) = h(\mathbf{x}) + \epsilon(\mathbf{x})$$

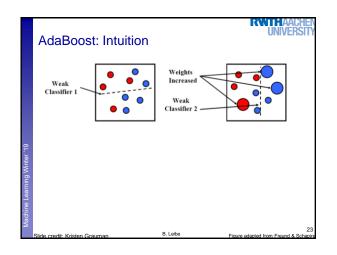
> Thus, the expected sum-of-squares error takes the form

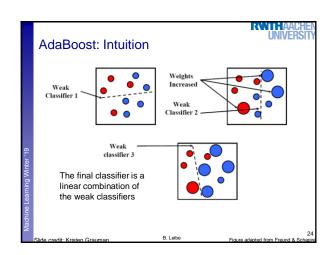
$$\mathbb{E}_{\mathbf{x}} = \left[\left\{ y_m(\mathbf{x}) - h(\mathbf{x}) \right\}^2 \right] = \mathbb{E}_{\mathbf{x}} \left[\epsilon_m(\mathbf{x})^2 \right]$$













AdaBoost – Formalization

- 2-class classification problem
 - Given: training set $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ with target values $\mathbf{T} = \{t_1, \ldots, t_N \}, t_n \in \{\text{-1,1}\}.$
 - Associated weights $\mathbf{W} = \{w_1, ..., w_N\}$ for each training point.
- Basic steps
 - ightarrow 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 x_n was misclassified by h_m(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,...,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.

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

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

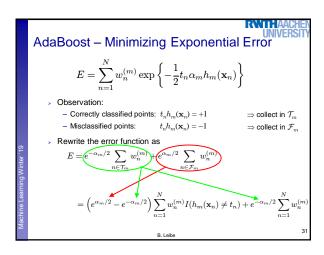
- Goal
 - Minimize E with respect to both the weighting coefficients α_l and the parameters of the base classifiers $h_l(\mathbf{x})$.

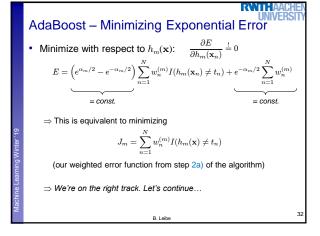
AdaBoost – Minimizing Exponential Error

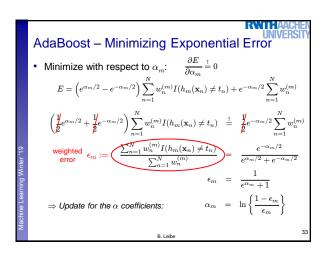
- Sequential Minimization
 - Suppose that the base classifiers $h_1(\mathbf{x}), \dots, h_{m-1}(\mathbf{x})$ and their coefficients $\alpha_{\mbox{\tiny 1}}, \ldots, \alpha_{\mbox{\tiny m--1}}$ are fixed.
 - \Rightarrow Only minimize with respect to α_m and $h_m(\mathbf{x}).$

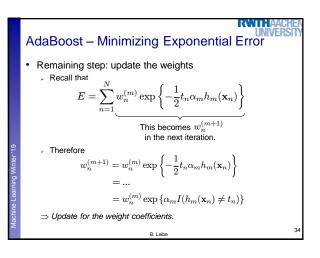
$$\begin{split} E &= \sum_{n=1}^{N} \exp\left\{-t_n f_m(\mathbf{x}_n)\right\} \quad \text{with} \quad f_m(\mathbf{x}) = \frac{1}{2} \sum_{l=1}^{m} \alpha_l h_l(\mathbf{x}) \\ &= \sum_{n=1}^{N} \exp\left\{-t_n f_{m-1}(\mathbf{x}_n) - \frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\} \\ &= \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\} \end{split}$$

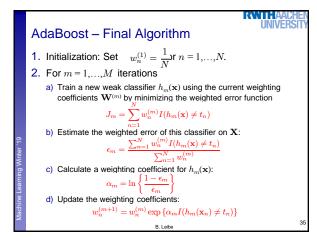
AdaBoost – Minimizing Exponential Error $E = \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2}t_n \alpha_m h_m(\mathbf{x}_n)\right\}$ Correctly classified points: t_nh_m(x_n) = +1 \Rightarrow collect in \mathcal{T} - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$ $E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m}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

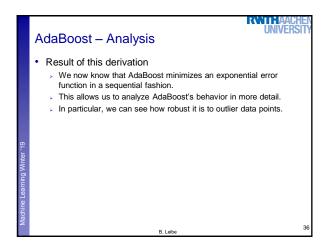


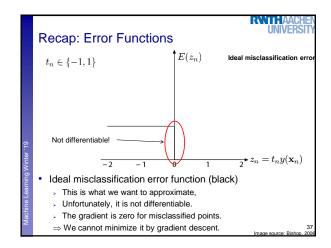


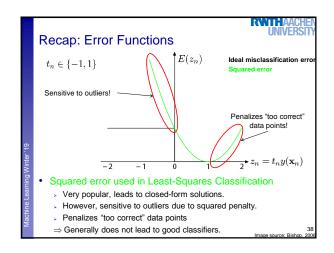


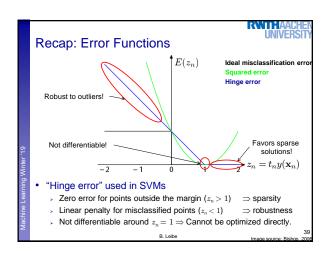


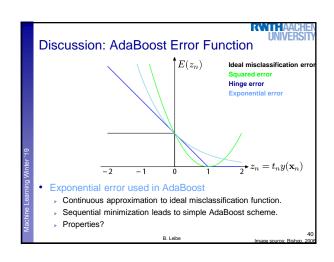


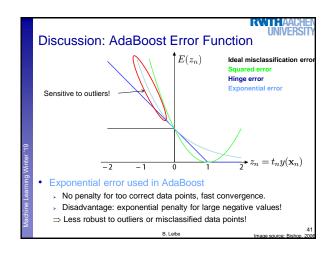


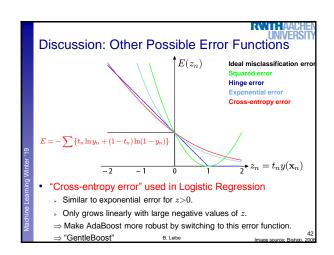












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Summary: AdaBoost

- 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



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 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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