

# Machine Learning 9 Bagging and Boosting

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https://www.ki.uni-stuttgart.de/

- Random forest based on slides by
  - Dr. Zeyd Boukhers, U. Koblenz-Landau



https://west.uni-koblenz.de/de/studying/courses/ws1718/machine-learning-and-data-mining-1



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#### **Learning Objectives**

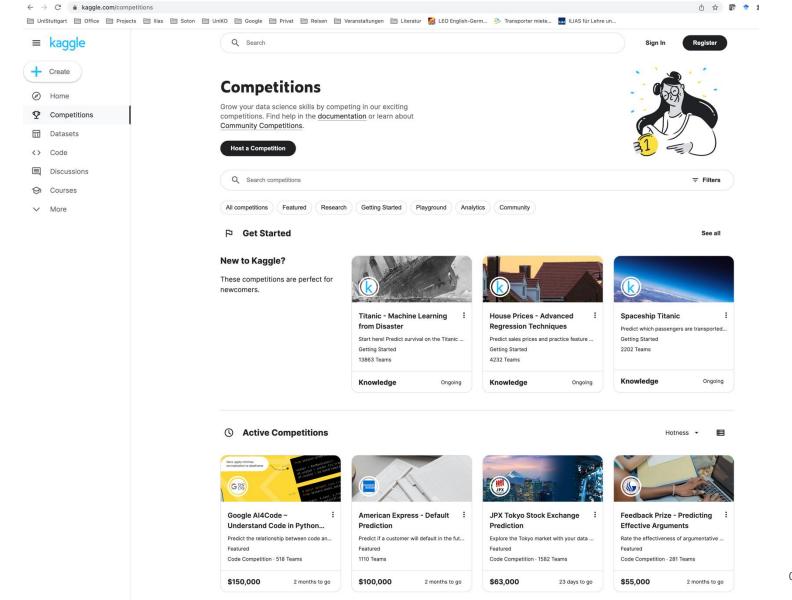
- Reconciling bias-variance trade-off by random forests
- Bagging Boostrap sampling
- AdaBoost
  - Properties of AdaBoost
- Gradient Boosting
- Power of weak learners
  - learning from uncorrelated data / methods
- Strengths and weaknesses of different loss functions
  - including exponential loss

# **Meaning of boxes**

explains the slide content

important take away

side note: nice to know



# Which machine learning methods win most Kaggle competitions?

- Not deep learning, but
- ensemble methods
  - previously: Random Forest
  - nowadays: XGBoost
  - maybe in the future: ensemble of neural networks
- Currently: XGBoost as the method to look to for tabular data
  - we do not consider XGBoost in this method,
     but it is a modification of Adaboost, which we consider

#### Reasons

- Table: (mostly) heterogeneous data
- Text / image: homogeneous data

- Deep learning: linear combinations (plus activation function) over homogeneous data
- Tree algorithms: individual treatments of table columns

# 1 Bagging and Boosting

#### **Prediction Error**

At an input  $x_0$  using squared error loss and a regression fit  $\hat{f}$  the prediction error is:

$$\operatorname{Err}(x_0) = E\left[\left(y_0 - \hat{f}(x_0)\right)^2\right] =$$

$$= E\left[\left(Y - \hat{f}(x_0)\right)^2 | X = x_0\right] =$$

$$= \sigma_{\varepsilon}^2 + \left[E\hat{f}(x_0) - f(x_0)\right]^2 + E\left[\hat{f}(x_0) - E\hat{f}(x_0)\right]^2 =$$

$$= \sigma_{\varepsilon}^2 + \operatorname{Bias}^2\left(\hat{f}(x_0)\right) + \operatorname{Var}\left(\hat{f}(x_0)\right) =$$

$$= \operatorname{Irreducible Error} + \operatorname{Bias}^2 + \operatorname{Variance}$$

Also cf. bias-variance trade-off in 4 Linear Regression

# What if variance of a prediction function is too high?

What if variance of a prediction function is too high?

For instance, decision trees tend to have small bias, but large variance

#### $\Rightarrow$ bagging

- 1. Choose data samples
- 2. Learn one predictor on this data sample
- 3. Regression: average the results of the predictors

  Classification: vote for classes by all the predictors

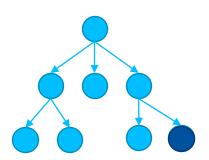
#### $\Rightarrow$ boosting

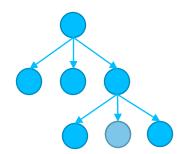
- 1. Iterate
  - (i) weight training data, (ii) choose weak predictor
- 2. Regression/Classification: weighted average of predictors

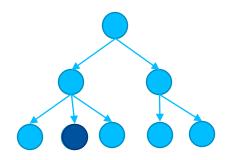
# 2 Constructing a Random Forest

#### Random forest

- It constructs multiple decision trees
- The final decision is made based on the majority votes of all trees.







#### Reducing variance

- Averaging B independent identically distributed (i.i.d.) random variables each with mean  $\mu$  and variance  $\sigma^2$  results in
  - mean  $\mu$  (this means: unchanged bias)
  - variance  $\frac{1}{R}\sigma^2$  (this means: lower variance)

• If random variables are pairwise correlated with  $\rho$ , new variance will be

$$\left(\rho + \frac{1-\rho}{B}\right)\sigma^2$$

### Bagging (also bootstrap aggregation)

- What if variance of a prediction function is too high?
- $\Rightarrow$  bagging
  - 1. Choose data samples
  - 2. Learn a predictor on every data sample
  - 3. Regression: average the results of the predictors Classification: vote for classes by all the predictors

⇒ random forests as a special method for bagging <u>uncorrelated</u> trees

#### Random forest

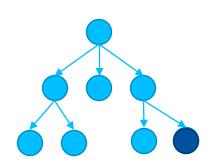
- Define the number of trees B
- For b = 1 to B
  - Draw a bootstrap sample  $Z^*$  of size  $N^*$  from the original data set with size N.
    - \*Bootstrap: random sampling with replacement.
  - Grow a random-forest tree  $T_b$  using the  $Z^*$  sample. For each node, repeat until minimal node size  $n_{min}$  is reached:
    - Select l\* attributes at random from all attributes.
    - Using Gain Ratio, split the node into children nodes.
- Output the ensemble of trees  $\{T_b\}_{b=1}^B$

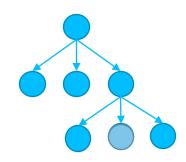
 $l^* < \sqrt{l}$ , even 1 uncorrelates the trees

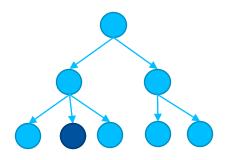
### Using random forest for classification

• Let  $\hat{f}_b(x)$  be the class prediction of x by the b tree,

$$\hat{f}(\mathbf{x}) = \underset{i}{\operatorname{argmax}} \sum_{b=1}^{D} [\hat{f}_b(\mathbf{x}) = i]$$







#### Generalization Error of an ensemble of Decision Trees

#### Notes:

- The bias of the ensemble is identical to the bias of a randomized tree but higher than the bias of a non-randomized tree.
- Stronger randomization:  $var(X) \rightarrow 0$
- Weaker randomization: var(X) → the variance of a non-randomized tree.

- ✓ Randomization increases bias but decreases the variance of the ensemble of trees.
  - ✓ Find the right bias-variance trade-off.

#### **Advantages**

- Better accuracy than a decision tree.
- Robustness to outliers and missing data.
- Robustness to irrelevant attributes.
- Non-parametric (completely random)
- Invariant to feature scaling and types.
- Reduces overfitting.
- High accuracy, especially for large data sets.

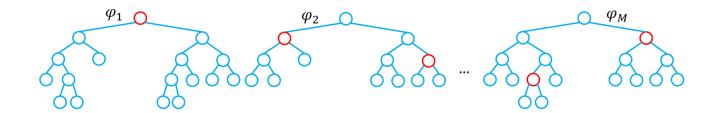
Interpretability ???

# 3 Interpreting Random Forests

# **Attribute importance score: Mean Decrease of Accuracy**

- Consider the out-of-bag samples (which were not sampled in the bootstrapped set).
  - Of course, we may use a separate set.
- Consider the corresponding trees.
- Permute the value of the attribute (to be assessed) with random noise.
- Consider an evaluation metric (e.g. accuracy)
- Compute the mean decrease of accuracy over all corresponding trees.
  - ➤ The attribute is important when the MDA is high

### Attribute importance score: Mean Decrease of Impurity



Importance of variable  $X_i$  for an ensemble of B trees  $\phi_m$  is :

$$\operatorname{Imp}(X_j) = \frac{1}{B} \sum_{m=1}^{B} \sum_{t \in \varphi_m} 1(j_t = j) \Big[ p(t) \Delta i(t) \Big],$$

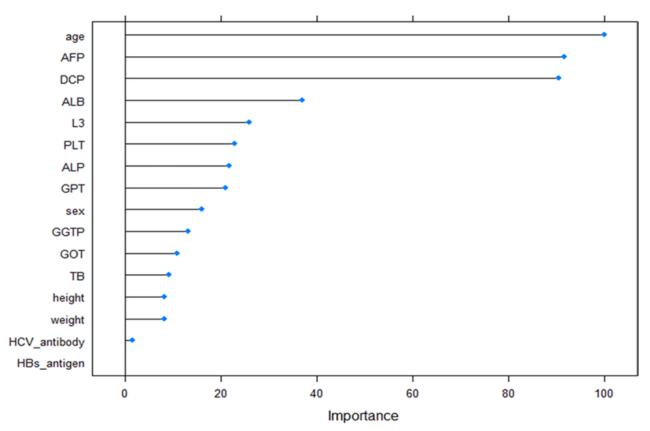
where  $j_t$  denotes the variable used at node t,  $p(t) = N_t/N$  and  $\Delta i(t)$  is the impurity reduction at node t:

$$\Delta i(t) = i(t) - \frac{N_{t_L}}{N_t} i(t_L) - \frac{N_{t_r}}{N_t} i(t_R)$$

# **Attribute importance scores (2)**

- Mean Decrease in Impurity (MDI):
  - The importance of an attribute  $x_i$  is measured as:
    - $Imp(x_j) = \frac{1}{B} \sum_{b=1}^{B} \sum_{t:b(t)=x_j} P(t) * \Delta I(t),$
    - Where  $P(t) = \frac{N_t}{N}$
  - The intuition is that an attribute is important when:
    - It decreases many impurities
    - It is used to split nodes with many samples.
    - It is used many times.
- Compared to MDA, MDI is widely used because:
  - It is faster and easier to compute.
  - Experiences showed that it correlates well with MDA.

# **Example of MDI**



Source: Sato, M., Morimoto, K., Kajihara, S., Tateishi, R., Shiina, S., Koike, K., & Yatomi, Y. (2019). Machine-learning Approach for the Development of a Novel predictive Model for the Diagnosis of Hepatocellular Carcinoma. *Scientific reports*, 9.

### **Computational complexity**

	Training	Prediction
Decision Tree	$O(l * N \log^2(N))$	O(l)
Random Forest	$O(B * \hat{l} * \widehat{N} \log^2(\widehat{N}))$	$O(B * \hat{l})$
Extra Tree	$O(B * \hat{l} * N \log(N))$	$O(B*\hat{l})$

- $\hat{l}$ : the number of variables randomly drawn at each node.
- *B*: the number of trees
- $\hat{N} = 0.632N$

# Take away

#### On random forests

 Sampling the data is not good enough, sampling of attributes is also needed

#### In general

- When approaching a new machine learning problem:
  - try simple methods first
  - random forest is a very good simple method to start with

# 4 Explainable Machine Learning

### Local feature attributions by Shapley values

Coalition game theory: allocate the surplus generated by grand coalition to players

The Shapley value  $S_j$  for the j 'th player is defined via a

$$S_j(\text{val}) = \sum_{T \subseteq N \setminus \{j\}} \frac{|T|! (p - |T| - 1)!}{p!} (\text{val}(T \cup \{j\}) - \text{val}(T))$$

- $N = \{1, ..., p\}$  is the set of features; x is the vector of the instance to be explained,
- $\operatorname{val}_{f,x}(T)$  represents the prediction for the feature values in T that are marginalized over features that are not included in T:

val: 
$$2^N \to \mathbb{R}$$
, val<sub>f,x</sub> $(T) = E_{X|X_T = x_T}[f(X)] - E_X[f(X)]$ 

### **Properties of Shapley values**

#### **Efficiency Property.**

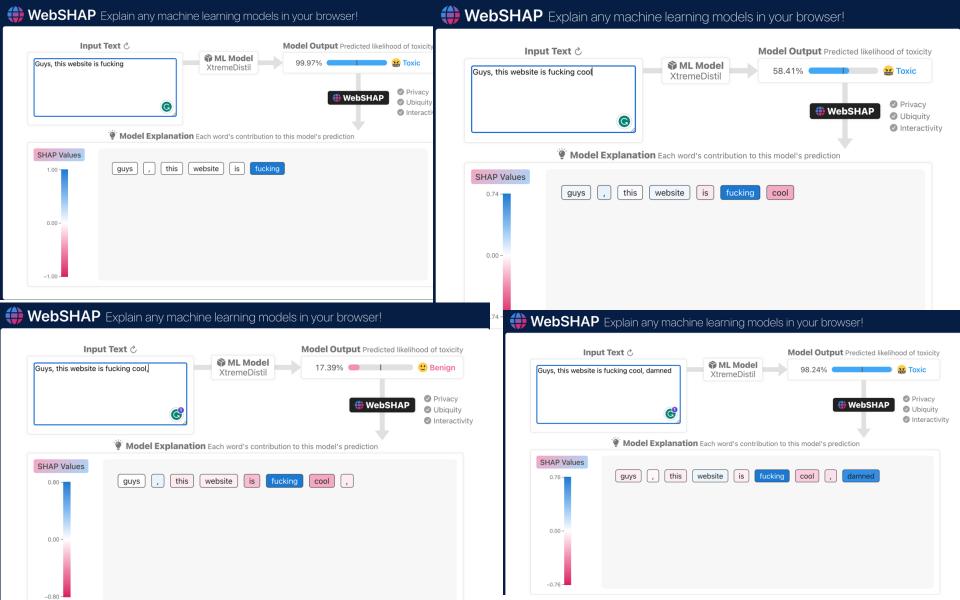
Feature contributions add up to the difference of prediction from  $x^*$  and the expected value:

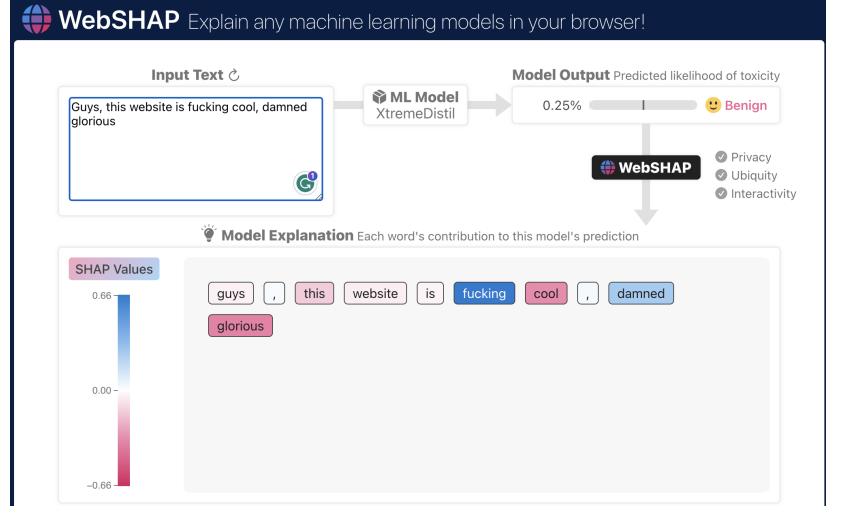
$$\sum_{j \in N} S_j(f, x^*) = f(x^*) - E[f(X)]$$

#### **Uninformativeness Property.**

A feature *j* that does not change the predicted value has a Shapley value of zero.

$$\forall x, x_j, x_i' : f(\{x_{N\setminus\{j\}}, x_i\}) = f(\{x_{N\setminus\{j\}}, x_i'\}) \Rightarrow \forall x : S_j(f, x) = 0$$





https://arxiv.org/abs/2303.09545

# **5 Decision Stumps**

#### A Tree with Two Branches: Decision stump

- Training data  $\{(x_i, y_i)\}_{i=1}^N$  with  $x_i \in \mathbb{R}^d$  and  $y_i \in \{-1,1\}$
- A decision stump is a function  $\phi_{j,s}$ , which is parametrized by
  - polarity  $p \in \{-1,1\}$
  - threshold  $s \in \mathbb{R}$
  - index  $j \in [1,2,...d]$

$$\phi_{j,s}(x_{\cdot}) = p \operatorname{sign}(x_{\cdot,j} - s) = \begin{cases} p, \text{ if } x_{\cdot,j} \ge s \\ -p, \text{ otherwise} \end{cases}$$

### Select best decision stump

Error of decision stump

$$\widehat{Err}(\phi_{j,s}) = \frac{1}{N} \sum_{i=1}^{N} [\phi_{j,s}(x_i) \neq y_i] =$$

$$= \frac{1}{N} \sum_{i=1}^{N} [y_i(x_{i,j} - s) \leq 0]$$

Determine

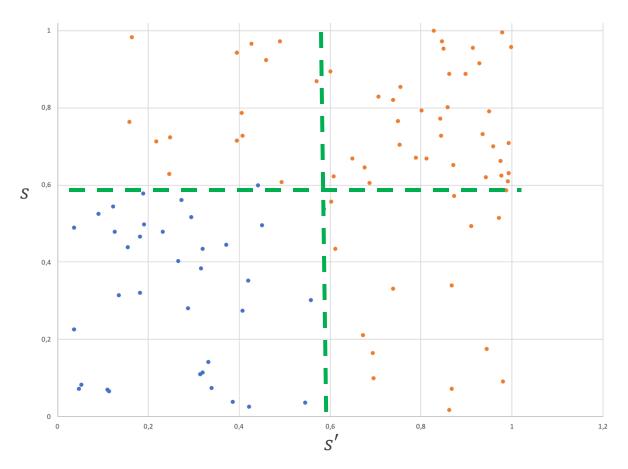
$$\underset{j \in \{1,\dots,d\}, s \in \{x_{i,j} | i \in \{1,\dots,N\}\}}{\operatorname{argmin}} \widehat{Err}(\phi_{j,s})$$

Intuitively: a decision stump selector is a weak learner (with large training error)

# **Examples for decision stumps**

$$\phi_{2,s}(x) = \operatorname{sign}(x_{\cdot,2} - s)$$

$$\phi_{1,s'}(x) = \operatorname{sign}(x_{\cdot,1} - s')$$



#### Other weak learners

- Selection from nominal features
- Selection from categorial features
- Decision trees
  - of limited depth

# **6 AdaBoost**

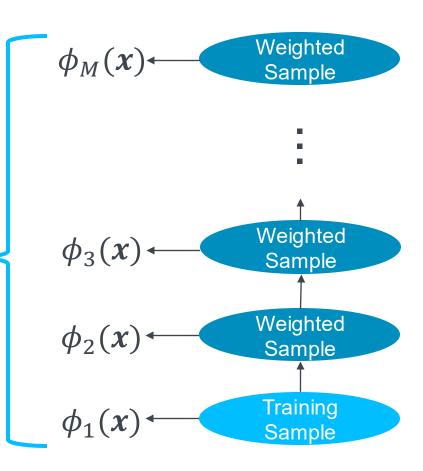
#### AdaBoost Scheme: Weighting data, weighting feature functions

- Assume infinite collection of feature functions  $\phi_i \colon \mathbb{R}^d \to \{-1,1\}$
- Assume infinite vector  $\theta = [\theta_1 \ \theta_2 \dots]^T$  with finite number of non-zero entries
- Classifier:

$$\hat{f}_{\theta}(\mathbf{x}) = \operatorname{sign}\left(\sum_{j=1}^{\infty} \theta_j \phi_j(\mathbf{x})\right)$$

• We also write  $\sum_{j=1}^{\infty} \theta_j \phi_j(x) = \theta^T \phi(x)$ 

How to select  $\theta$  and  $\phi(x)$ ?



#### Discrete AdaBoost Algorithm

1. Init weights  $w_i = \frac{1}{N}$  for  $i = 1 \dots N$ 

#### 2. Repeat

Could be decision stump  $\phi_{j,s}(x)$ 

- a. Fit a classifier  $\phi_m(x)$  to the training data using weights  $w_i$
- b. Compute normalized weighted error

$$\widehat{Err}(\phi_m) = \frac{\sum_{i=1}^N w_i \left[\phi_m(x_i) \neq y_i\right]}{\sum_{i=1}^N w_i}$$

- c. Compute log odds  $\theta_m = \log \frac{1 \widehat{Err}(\phi_m)}{\widehat{Err}(\phi_m)}$
- d. Set  $w_i := w_i \cdot e^{\theta_m[y_i \neq \phi_m(x_i)]}$  for  $i = 1 \dots N$

**Until** convergence of  $\theta^T \phi(x)$ 

3. Output  $\hat{f}(x) = \text{sign}[\theta^T \phi(x)]$ 

#### Side note:

"Real AdaBoost" is a regression method

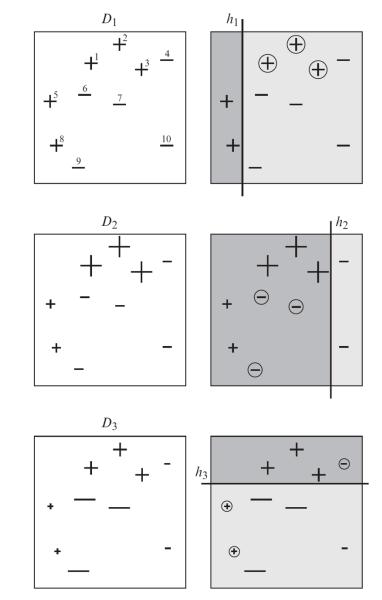
#### **Illustration of AdaBoost**

Each row depicts one round.

The left box in each row represents the training data, with the size of each example scaled in proportion to its weight.

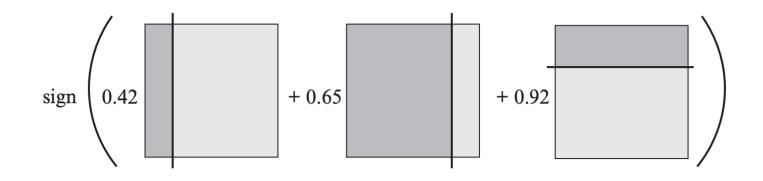
Each box on the right shows the weak hypothesis  $\phi_m$ , where darker shading indicates the region of the domain predicted to be positive.

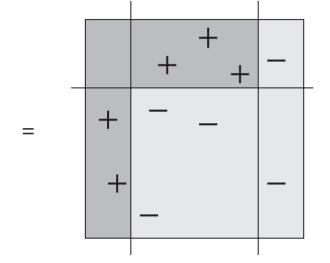
Examples that are misclassified by  $\phi_m$  have been circled.



(Schapire, R. E. and Freund, Y. 2012), Figure 1.1.

# Combined $\phi_m$

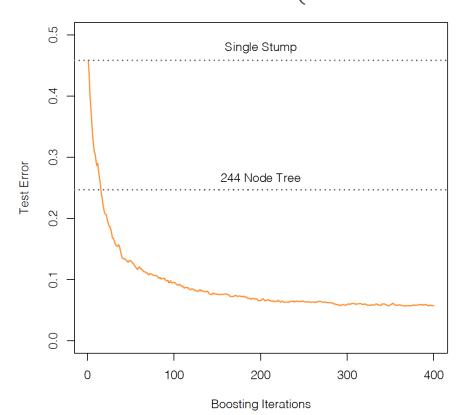




(Schapire, R. E. and Freund, Y. 2012), Figure 1.2.

#### **Artificial Example: Sum of squares of 10 standard Gaussians**

Artificial data 
$$Y = \begin{cases} 1, & \text{if } \sum_{j=1}^{10} X_j^2 > \chi_{10}^2 (0.5) = 9.34 \\ -1, & \text{else} \end{cases}$$



- Single decision stump hardly better than random
- 400 combined stumps much better than a single large decision tree (error rate 24.7%)

(Hastie et al; Figure 10.2)

# 7 Understanding AdaBoost

#### **Boosting Fits an Additive Model**

Assume basis functions  $b(x; \beta_m)$ 

$$\hat{f}(x) = \sum_{m=1}^{\infty} \theta_m b(x; \beta_m)$$

where

 $\theta_m$  are the expansion coefficients and

 $\beta_m$  are the parameters

Side note: Additive expansions are at the core of many learning techniques

- single hidden-layer neural networks
- signal processing: wavelets or sinus functions as base functions
- multivariate adaptive regression splines

#### What should be avoided

Do not aim at global optimization of loss

$$\underset{\{\theta_m,\beta_m\}_1^M}{\operatorname{argmin}} \sum_{i=1}^N L\left(y_i, \sum_{m=1}^\infty \theta_m b(x_i; \beta_m)\right)$$

- Computationally too expensive
- Instead: Fit one basis function at a time!

### Algorithm: Foreward Stagewise Additive Modeling

- 1. Initialize  $\hat{f}_0(x) = 0$
- 2. Repeat until convergence
  - a. Compute

$$(\theta_m, \beta_m) = \underset{\widetilde{\theta}, \widetilde{\beta}}{\operatorname{argmin}} \sum_{i=1}^N L(y_i, \hat{f}_{m-1}(x_i) + \widetilde{\theta}b(x_i; \widetilde{\beta}))$$

b. Incrementally set

$$\hat{f}_m(x) = \hat{f}_{m-1}(x) + \theta_m b(x_i; \beta_m)$$

#### AdaBoost and Forward Stagewise Additive Modeling

- What is the connection between AdaBoost and Forward Stagewise Additive Modeling?
- Which loss function is used by AdaBoost?
- Exponential loss:

 $L\left(y,\hat{f}(x)\right) = e^{-y\hat{f}(x)}$ 

It took the community 5 years to find this result

Solve

$$(\theta_m, \phi_m) = \underset{\widetilde{\theta}, \widetilde{\phi}}{\operatorname{argmin}} \sum_{i=1}^N e^{-y_i (\hat{f}_{m-1}(x_i) + \widetilde{\theta} \widetilde{\phi}(x_i))}$$

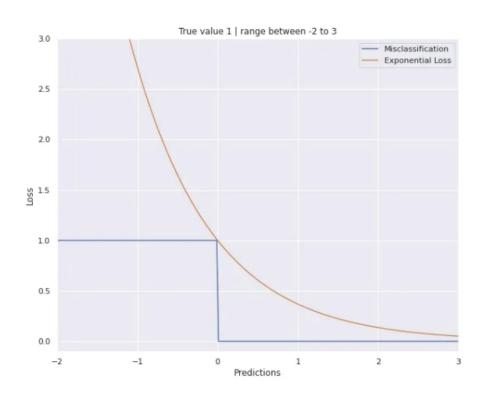
#### **Exponential loss**

def exponential\_loss(y\_pred, y\_true):
 return np.mean(np.exp(- y\_pred \* y\_true))

VS

The result can be shown below:

#### 0-1-loss



### AdaBoost and Forward Stagewise Additive Modeling

- Exponential loss:  $L(y, \hat{f}(x)) = e^{-y\hat{f}(x)}$
- Solve

$$(\theta_{m}, \phi_{m}) = \underset{\widetilde{\theta}, \widetilde{\phi}}{\operatorname{argmin}} \sum_{i=1}^{N} e^{-y_{i} (\hat{f}_{m-1}(x_{i}) + \widetilde{\theta} \widetilde{\phi}(x_{i}))} =$$

$$= \underset{\widetilde{\theta}, \widetilde{\phi}}{\operatorname{argmin}} \sum_{i=1}^{N} e^{-y_{i} \hat{f}_{m-1}(x_{i})} e^{-y_{i} \widetilde{\theta} \widetilde{\phi}(x_{i})} = \underset{\widetilde{\theta}, \widetilde{\phi}}{\operatorname{argmin}} \sum_{i=1}^{N} w_{i}^{(m)} e^{-y_{i} \widetilde{\theta} \widetilde{\phi}(x_{i})}$$

• For any  $\tilde{\theta} \ge 0$  this is equivalent to:

$$\underset{\widetilde{\theta},\widetilde{\phi}}{\operatorname{argmin}} \sum_{i=1}^{N} w_{i}^{(m)} \left[ y_{i} \neq \widetilde{\phi}(x_{i}) \right]$$

because...

remember the

#### Proving the claim: Relating exponential loss and weighted error

Proving the claim: 
$$\tilde{\theta} = \frac{1}{2} \log \frac{\left(1 - \widehat{Err}(\tilde{\phi})\right)}{\widehat{Err}(\tilde{\phi})}$$

$$\frac{\partial(e^{\widetilde{\theta}} - e^{-\widetilde{\theta}})\widehat{Err}(\widetilde{\phi}) + e^{-\widetilde{\theta}}}{\partial\widetilde{\theta}} = (e^{\widetilde{\theta}} + e^{-\widetilde{\theta}})\widehat{Err}(\widetilde{\phi}) - e^{-\widetilde{\theta}} = \mathbf{0}$$

$$\widehat{Err}(\widetilde{\phi})e^{\widetilde{\theta}} - (1 - \widehat{Err}(\widetilde{\phi}))e^{-\widetilde{\theta}} = 0$$

$$\widehat{Err}(\widetilde{\phi})e^{\widetilde{\theta}} = (1 - \widehat{Err}(\widetilde{\phi}))e^{-\widetilde{\theta}}$$

$$\widetilde{\theta} + \log\widehat{Err}(\widetilde{\phi}) = -\widetilde{\theta} + \log(1 - \widehat{Err}(\widetilde{\phi}))$$

$$2\tilde{\theta} = \log\left(1 - \widehat{Err}(\tilde{\phi})\right) - \log\widehat{Err}(\tilde{\phi}) = \log\frac{\left(1 - \widehat{Err}(\tilde{\phi})\right)}{\widehat{Err}(\tilde{\phi})}$$

#### 2a Updating in Forward Stagewise Additive Modeling

$$\hat{f}_m(x) = \hat{f}_{m-1}(x) + \theta_m \phi_m(x)$$

#### Causing next weights to be

$$w_i^{(m+1)} = w_i^{(m)} \cdot e^{-y_i \theta_m \phi_m(x_i)} = w_i^{(m)} \cdot e^{\alpha_m [y_i \neq \phi_m(x_i)]} \cdot e^{-\theta_m}$$

use update like this

or bring it into form used by AdaBoost 2d,

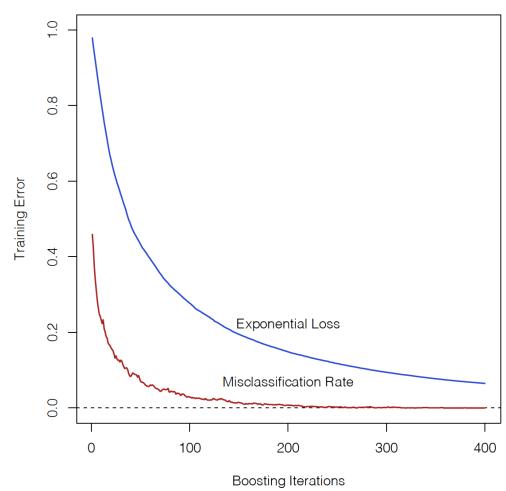
with 
$$\alpha_m = 2\theta_m$$

and  $e^{-\theta_m}$  a constant factor to all weights that is therefore ignored

# 8 Understanding Losses

# Artificial Example: Sum of squares of 10 standard Gaussians

- After 250 iterations the training error is 0,
- but exponential loss continues to decrease



(Hastie et al), Figure 10.3

## Comparing loss functions for binary classification

Missclassification:

$$[sign(\hat{f}) \neq y]$$

Exponential:

$$e^{-y\hat{f}}$$

Cross entropy (binomial deviance):

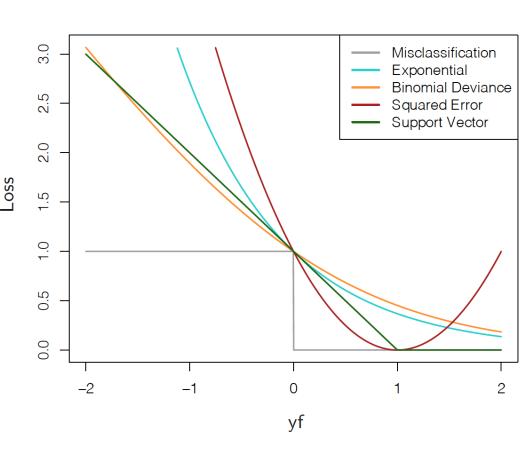
$$\log(1 + e^{-2y\hat{f}})$$

Squared error:

$$(y-\hat{f})^2$$

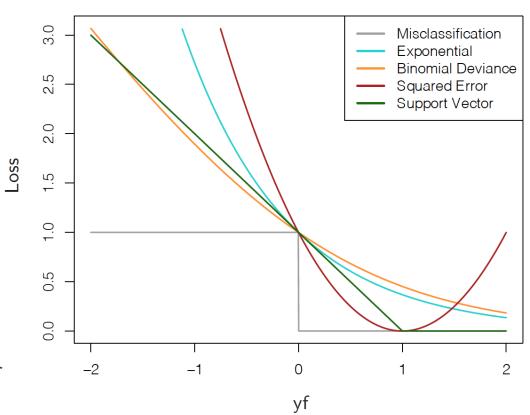
Hinge loss (support vector):

$$\max(0,1-y\hat{f})$$



#### Comparing loss functions for binary classification

- Squared error loss does not decrease continuously,
- ⇒ unnecessary attention on correctly classified entities
- Exponential loss punishes wrong predictions exponentially
- ⇒problematic when Bayes error is high
- ⇒ AdaBoost deteriorates in such settings
- Cross entropy and hinge loss deal better with high Bayes error in the data set



#### Comparing loss functions for regression

Squared error:

$$(y-\hat{f})^2$$

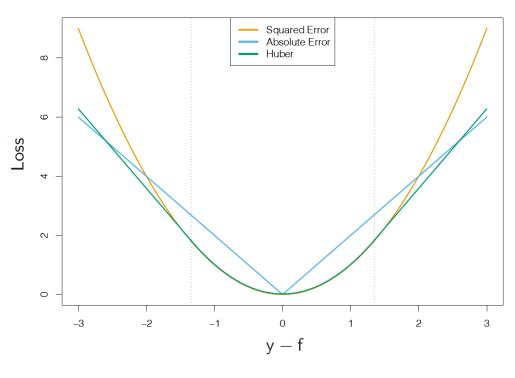
Absolute error

$$|y - \hat{f}|$$

Huber

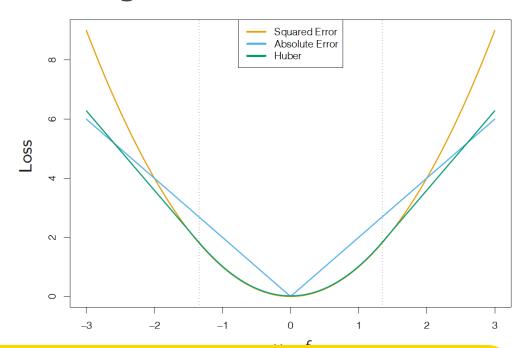
$$L\left(y,\hat{f}(x)\right) =$$

$$= \begin{cases} \left[ y - \hat{f}(x) \right]^2, & \text{for } |y - \hat{f}(x)| < \delta \\ 2\delta |y - \hat{f}(x)| - \delta^2, & \text{otherwise} \end{cases}$$



#### Comparing loss functions for regression

- Squared error loss emphasizes large absolute residuals  $|y \hat{f}|$
- ⇒ less robust against outliers
- ⇒ problematic with long-tailed error distributions



Some loss functions perform badly in certain situations,

- Example classification: Squared error loss and exponential loss for boosting
- Example *regression*: Squared error loss for linear regression but they lead to simple and elegant methods, which others don't



#### Thank you!



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