Ensemble Learning

Machine Learning Group, TU Berlin

Outline

- Decision Trees
- Resampling schemes
- Random Forests / Bagging
- Boosting
- Relation to SVMs and Learning Theory

Classification

Many approaches derive from a theory

- LDA, QDA: Bayes decision theory
- SVM: VC theory

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- Decision trees
- Ensemble methods

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- Iterative procedure can be represented by a tree.

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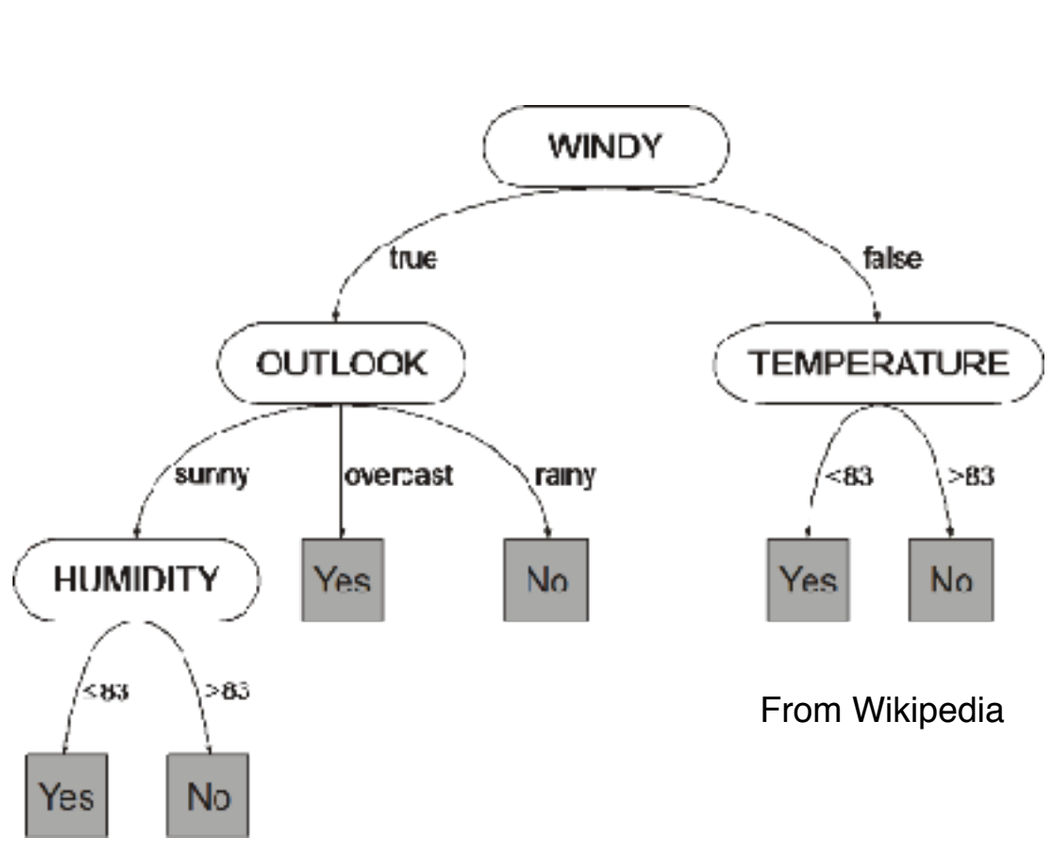

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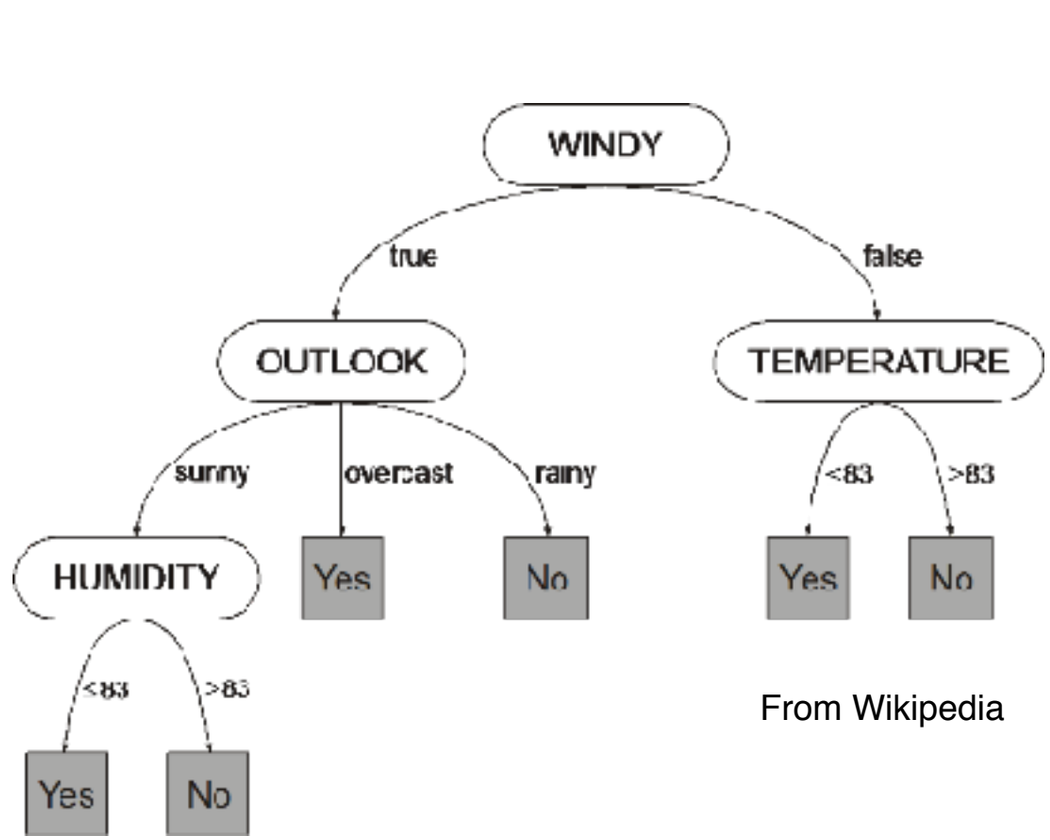

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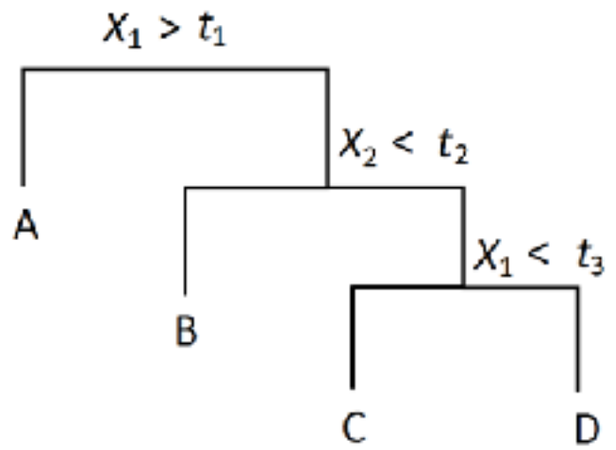
Decision trees

Formal definition

- Each leaf corresponds to a value of the target variable *y*
  - Categorial case: classification
  - Continuous case: regression

- Each interior node corresponds to a data dimension (feature) x_i
- Edges correspond to decisions
- Features may occur multiple times

Defines recursive partitioning of the feature space.



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Decision trees

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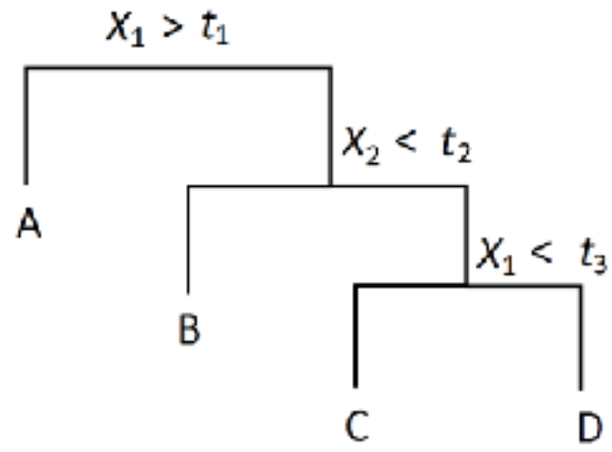

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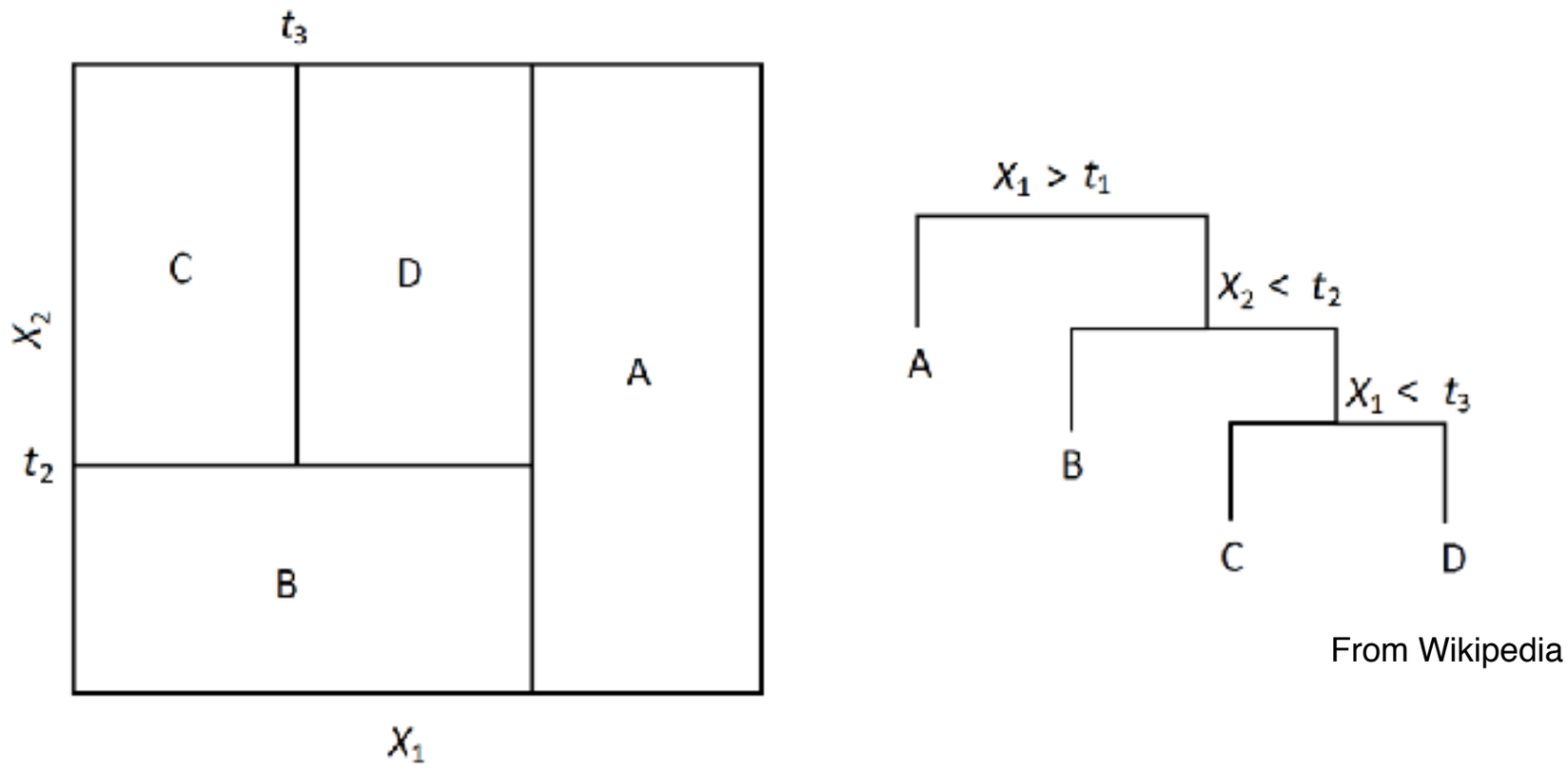
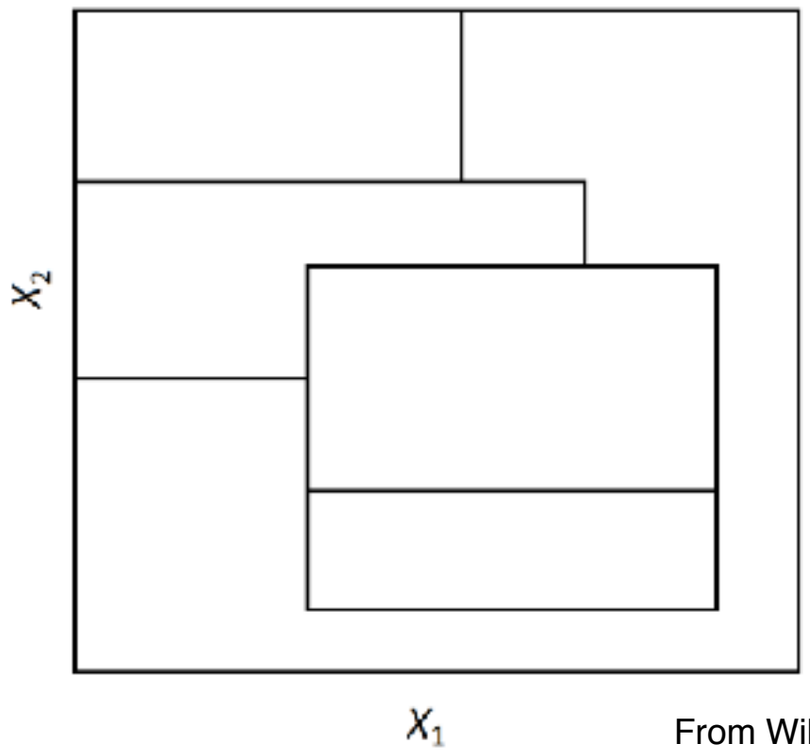


From Wikipedia

- Features treated separately → axes-parallel compartments.
- Nevertheless, can represent (arbitrary) complex functions.

Decision trees

What tree represents these decision boundaries?



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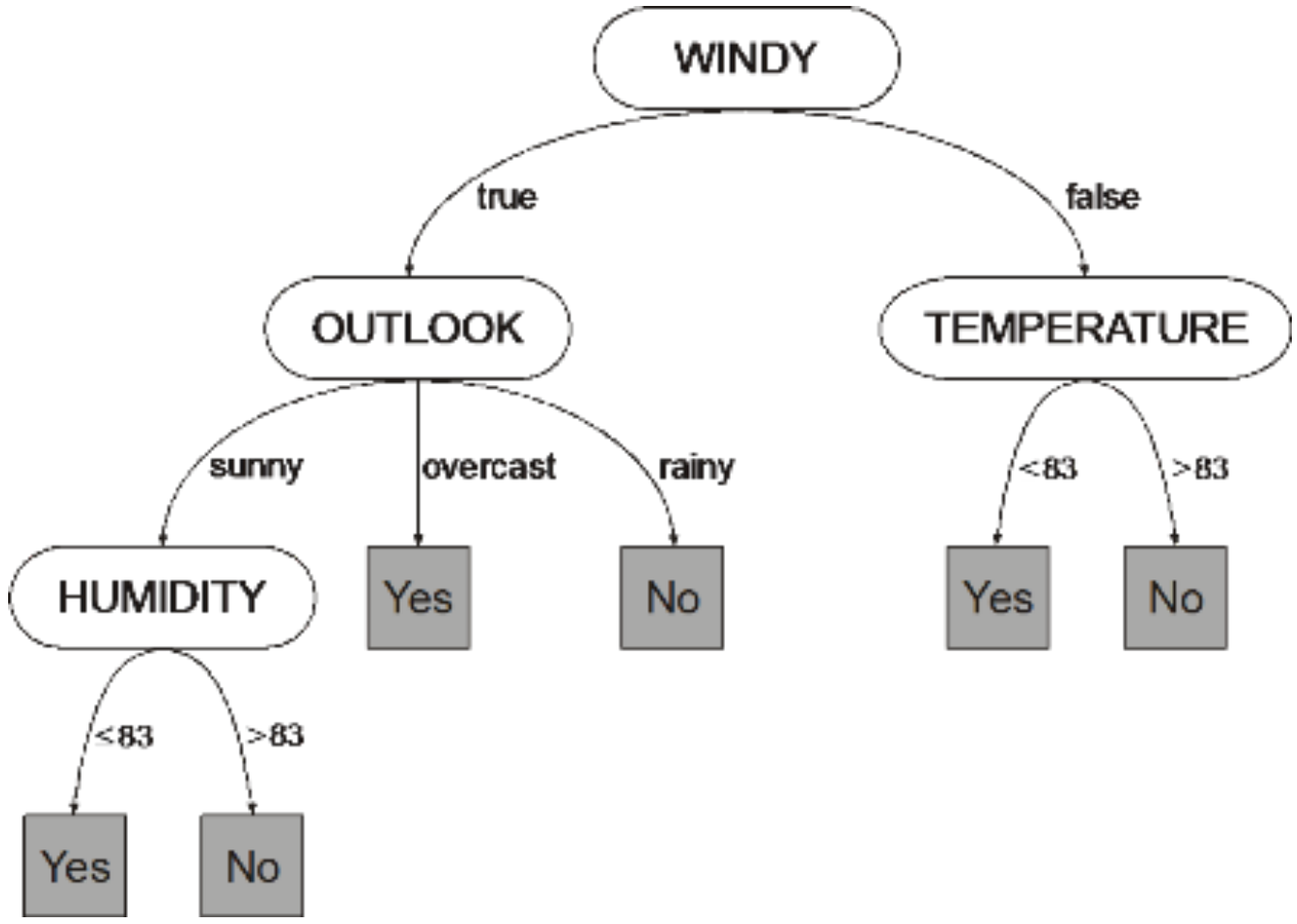
Possible to construct one, but requires many splits of the same features.

Predicting from a given tree



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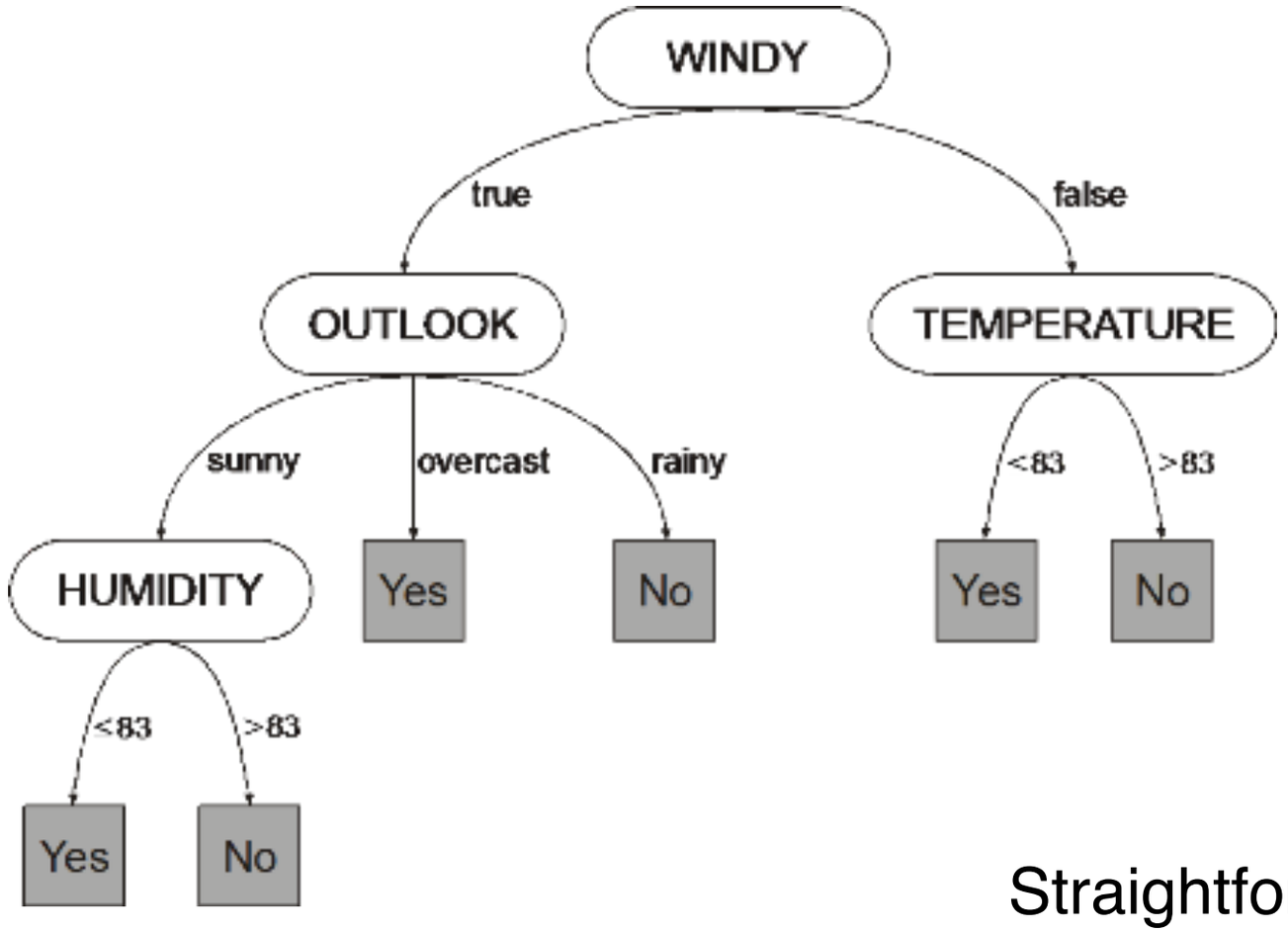

Straightforward

‘Growing’ a decision tree

- Many ways to choose splittings, order of variables.
- Low tree complexity leads to high generalization performance.

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→ Greedy approaches

- ID3/C4.5
- CART

ID3

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  - Select feature with largest information gain to split tree.
  - Recurse on subsets $\mathcal{T}_k$ using remaining features.
  - If no more feature exists, add leaf node for majority class and stop.

Splitting criterion

Entropy: measures the uncertainty in a set $\mathcal{X}$

$$H(\mathcal{X}) = -\sum_{c \in C} p(c) \log p(c) \qquad \text{, where}$$

- C is the set of classes occurring in $\mathcal{X}$
- p(c) is the proportion of samples $\mathcal{X}$ that are in class c
- Low Entropy: all samples in the same class
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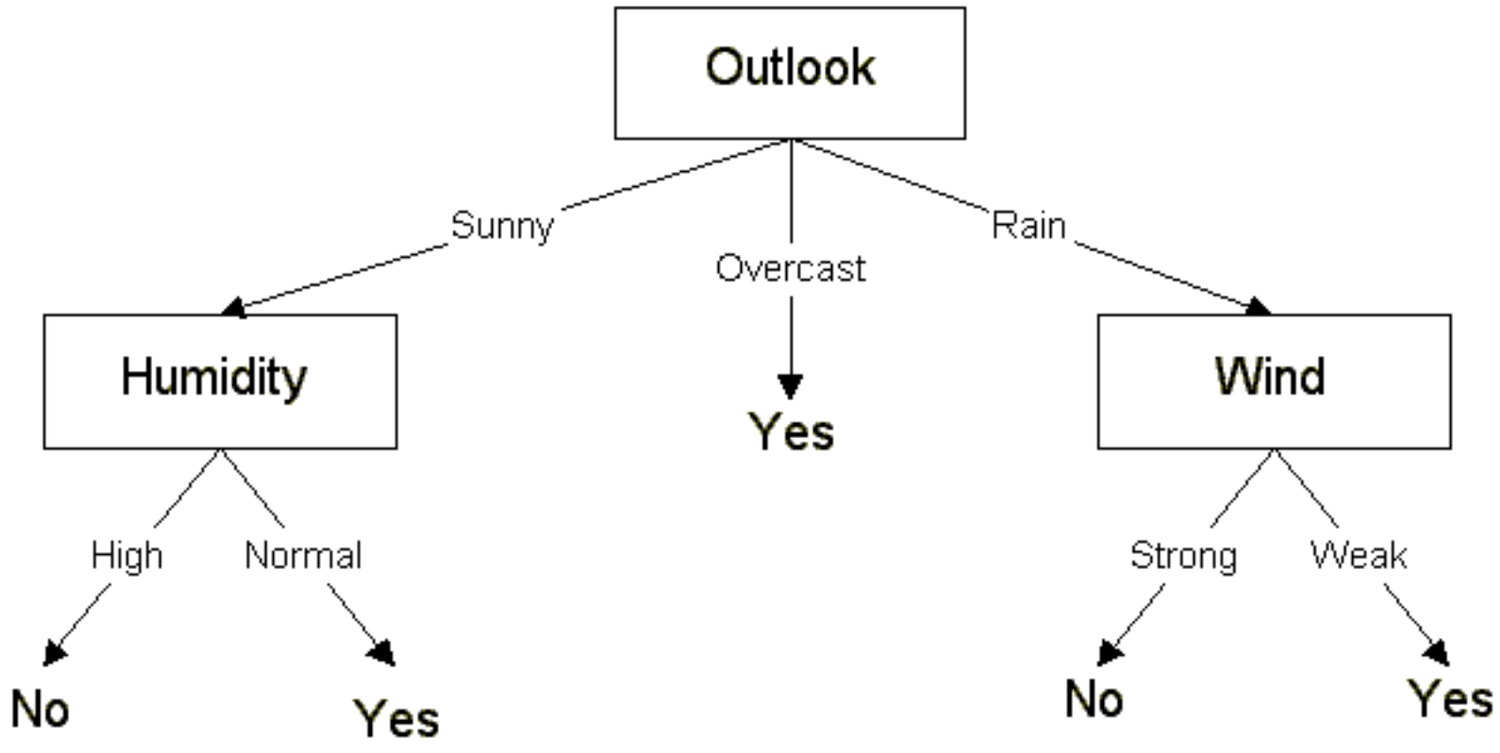
Information Gain:

$$IG(x_i, \mathcal{X}) = H(\mathcal{X}) - \sum_{k} p(\mathcal{T}_k) H(\mathcal{T}_k) \quad \text{, where}$$

- $p(\mathcal{T}_k)$ is the proportion of samples in $\mathcal{X}$ that are in $\mathcal{T}_k$.

Example

https://www.cise.ufl.edu/~ddd/cap6635/Fall-97/Short-papers/2.htm



C4.5

Extension of ID3 (Quinlan, 1993)

1. Handles continuous features by automatically setting a threshold base on maximal information gain.
2. Handles missing values.
3. Handles attributes with differing costs.
4. Pruning: Removes branches that do not help by replacing them with leaf nodes.
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   → 4 and 5 reduce overfitting.

CART

CART = Classification and Regression Trees (Leo Breiman, 1984)

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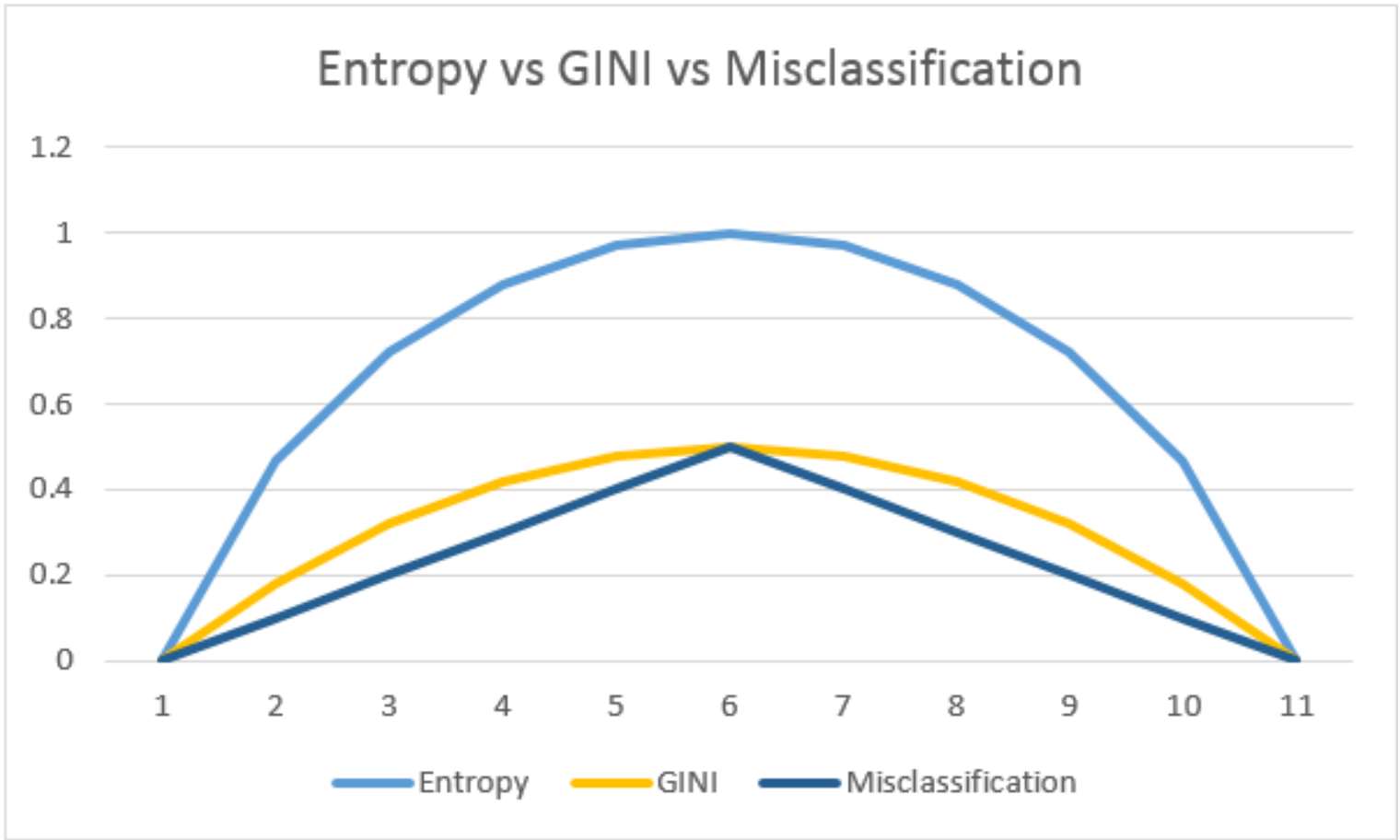
Classification: Gini Impurity — measures how often a randomly chosen sample from $\mathcal{X}$ would be incorrectly labeled if it was randomly labeled according to the distribution of labels in $\mathcal{X}$.

$$GI(\mathcal{X}) = \sum_{c=1}^{C} p(c)(1 - p(c)) = \sum_{c \neq \tilde{c}} p(c)p(\tilde{c})$$

→ Similar to entropy, zero if all samples belong to same class.

CART


Entropy vs GINI vs Misclassification
1.2
1
0.8
0.6
0.4
0.2
0
1
2
3
4
5
6
7
8
9
10
11
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CART

Regression: Variance reduction

$$VR(\mathcal{X}, x_i, h) = \text{Var}(\mathcal{X}) - \left(p(\mathcal{T}_n)\text{Var}(\mathcal{T}_n) + p(\mathcal{T}_p)\text{Var}(\mathcal{T}_p)\right) \text{, where}$$

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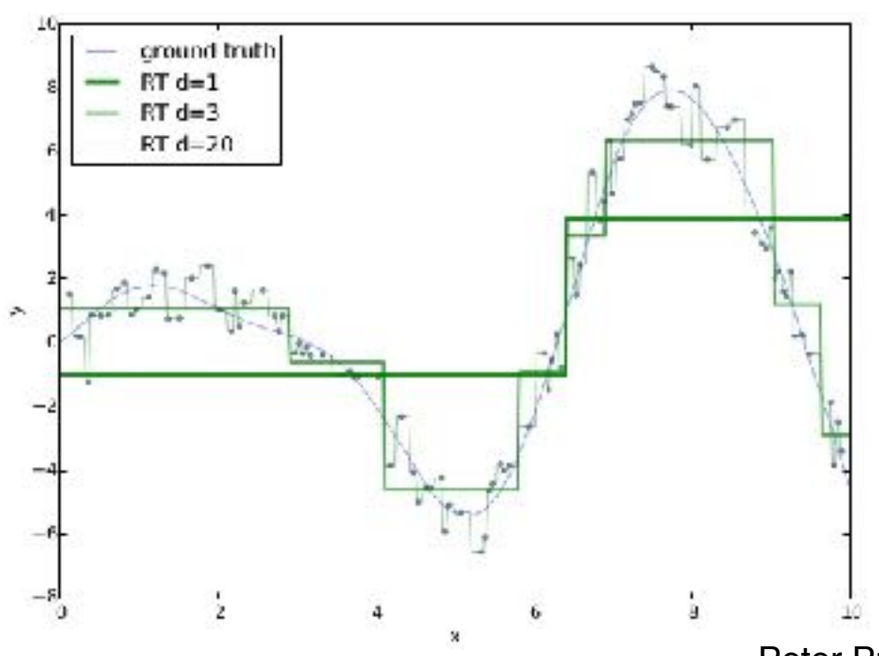

Peter Prettenhofer

Finiteness of tree leads to stepwise constant functions.

Advantages

- Simple to understand and interpret.
- Mirrors human decision making more closely than other approaches.
- Graphical representation.
- Non-parametric, few assumptions.
- Able to handle both numerical and categorical data.
- Requires little data preparation, no normalization/dummy variables.
- ‘White box’ model. Classification is easily explained by Boolean logic.
- Performs well with large datasets due to sequential univariate treatment.

Limitations

- Greedy, local optima.
- Non-robustness: small changes in training data and greedy strategy can change results.
- Overfitting, low test accuracy

  → Pruning
- Large trees needed to represent some simple functions (e.g. a sphere).

  → Multivariate Approaches (linear DT, PCA)
- No continuous regression.

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→ One solution for all problems: ensemble methods

Ensemble methods

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Motivation: ‘The Wisdom of Crowds’

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- 800 (lay) people guessed the weight of an ox at a country fair.
- Median guess deviated only 0.8% from the truth (mean even less).
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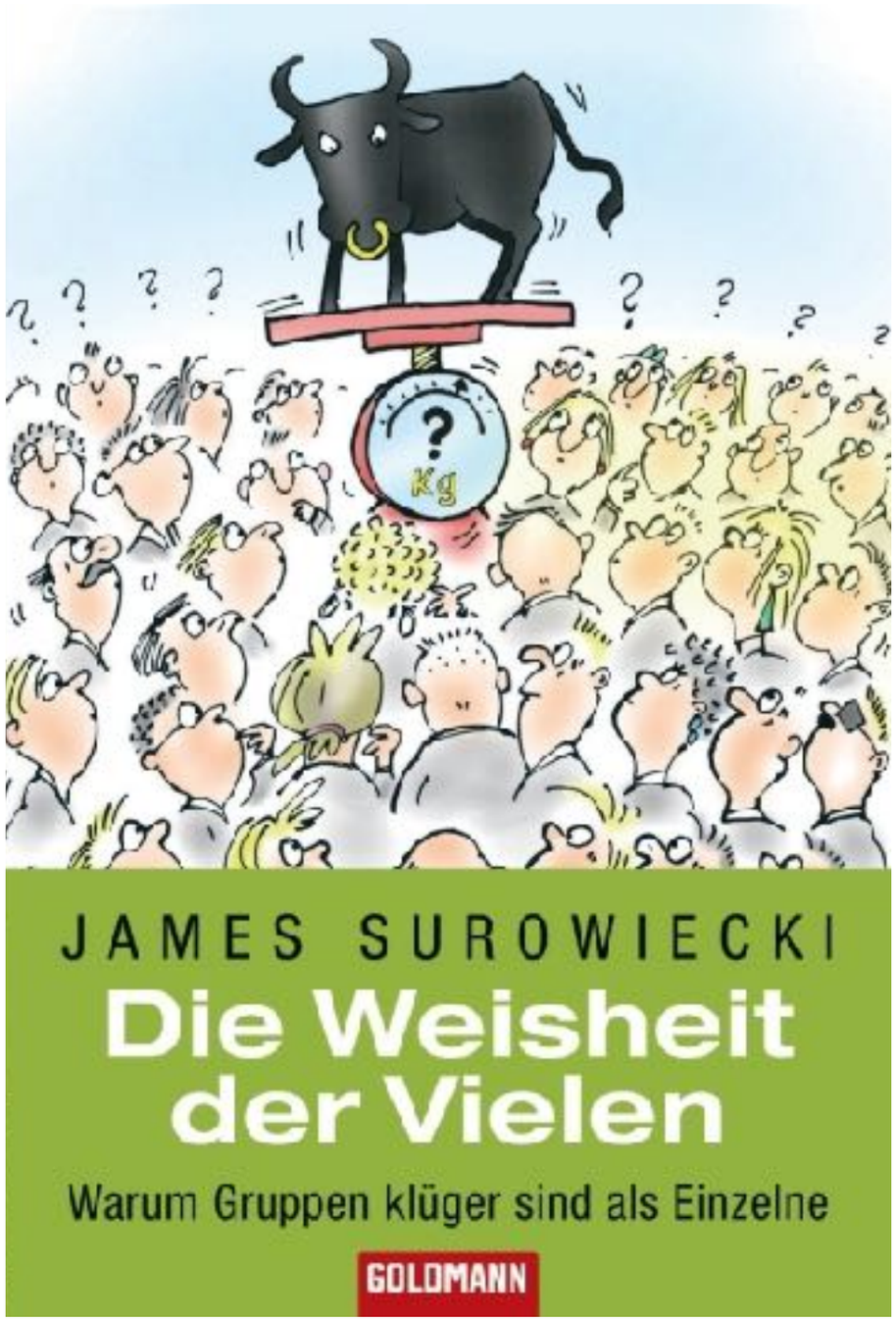

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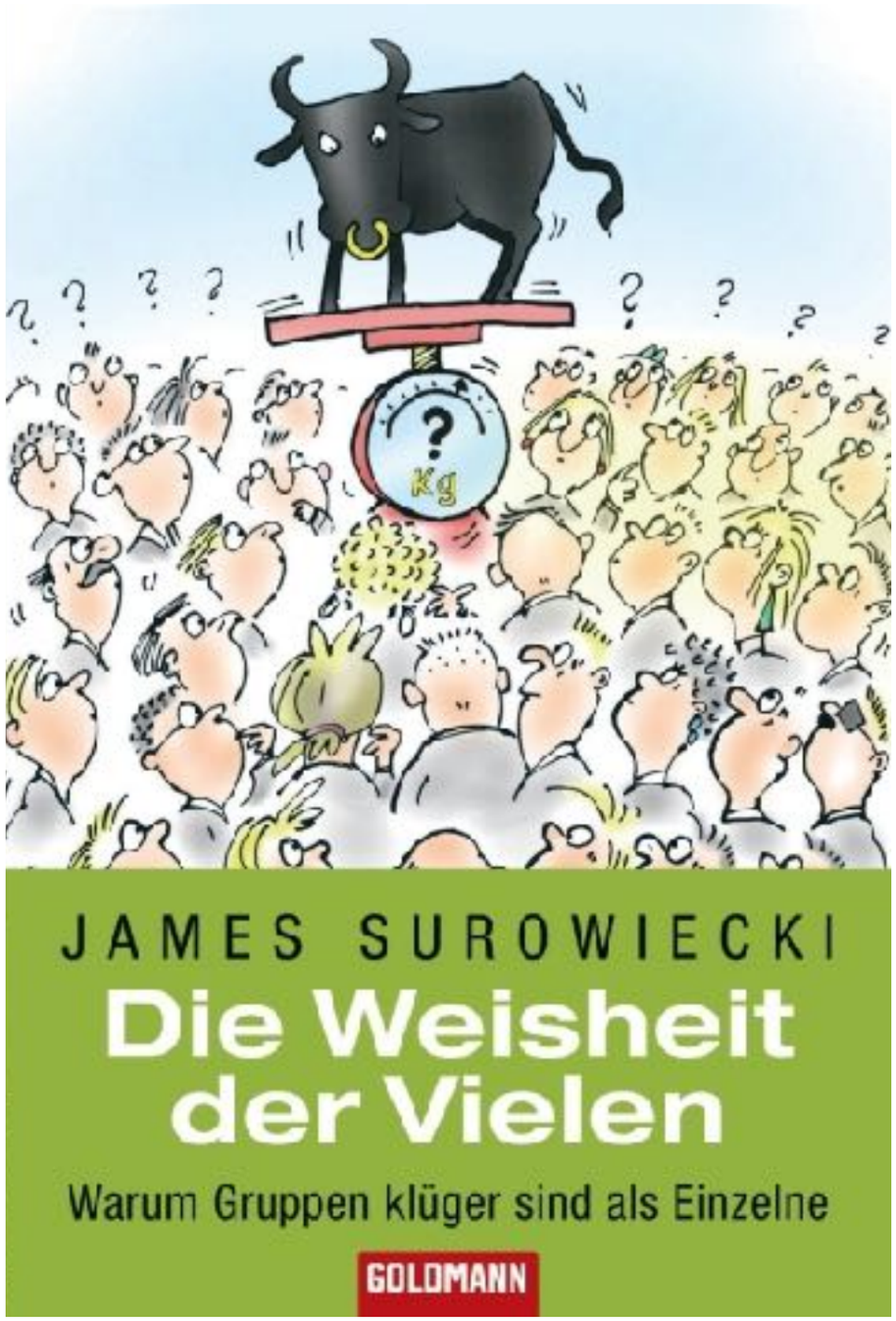

Example: mean

Mean: $\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} x_i$

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Using that variances are linear for independent x_i : $\mathrm{Var}(\sum_i x_i) = \sum_i \mathrm{Var}(x_i)$

$\mathcal{X}$

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→ **Resampling:** generate ‘new’ datasets by drawing samples from $\mathcal{X}$.

Jackknife (Maurice Quenouille, 1949)

Construct leave-one-out datasets $\mathcal{X}_i = \mathcal{X} \setminus \mathbf{x}_i$, $i \in \{1, \ldots, N\}$.

For any statistic θ, replace $\hat{\theta}(\mathcal{X})$ by Jackknife estimate $\hat{\theta}_J(\mathcal{X}) = \frac{1}{N} \sum_{i=1}^{N} \hat{\theta}(\mathcal{X}_i)$.

The variance of this estimator is $\mathrm{Var}\left[\hat{\theta}_J(\mathcal{X})\right] = \frac{N-1}{N} \sum_{i=1}^{N} \left(\hat{\theta}(\mathcal{X}_i) - \hat{\theta}_J(\mathcal{X})\right)^2$.

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Notes:

- $N - 1$ appears in the numerator, because the $\hat{\theta}(\mathcal{X}_i)$ are highly dependent.
- Jackknife estimators for the mean are identical to the usual $\hat{\mu}$ and $\hat{\sigma}^2/N$.
- But can be used for any statistic → very handy tool.
- Can also be used to estimate and remove the bias of $\hat{\theta}(\mathcal{X})$.

Bootstrap (Bradley Efron, 1979)

Construct new datasets $\mathcal{X}_i$, $|\mathcal{X}_i| = N$, $i \in \{1, \ldots, M\}$, by sampling from $\mathcal{X}$ with replacement.

Bootstrap estimate: $\hat{\theta}_B(\mathcal{X}) = \frac{1}{M} \sum_{i=1}^{M} \hat{\theta}(\mathcal{X}_i)$

Variance: $\text{Var}\left[\hat{\theta}_B(\mathcal{X})\right] = \frac{1}{M} \sum_{i=1}^{M} \left(\hat{\theta}(\mathcal{X}_i) - \hat{\theta}_B(\mathcal{X})\right)^2$

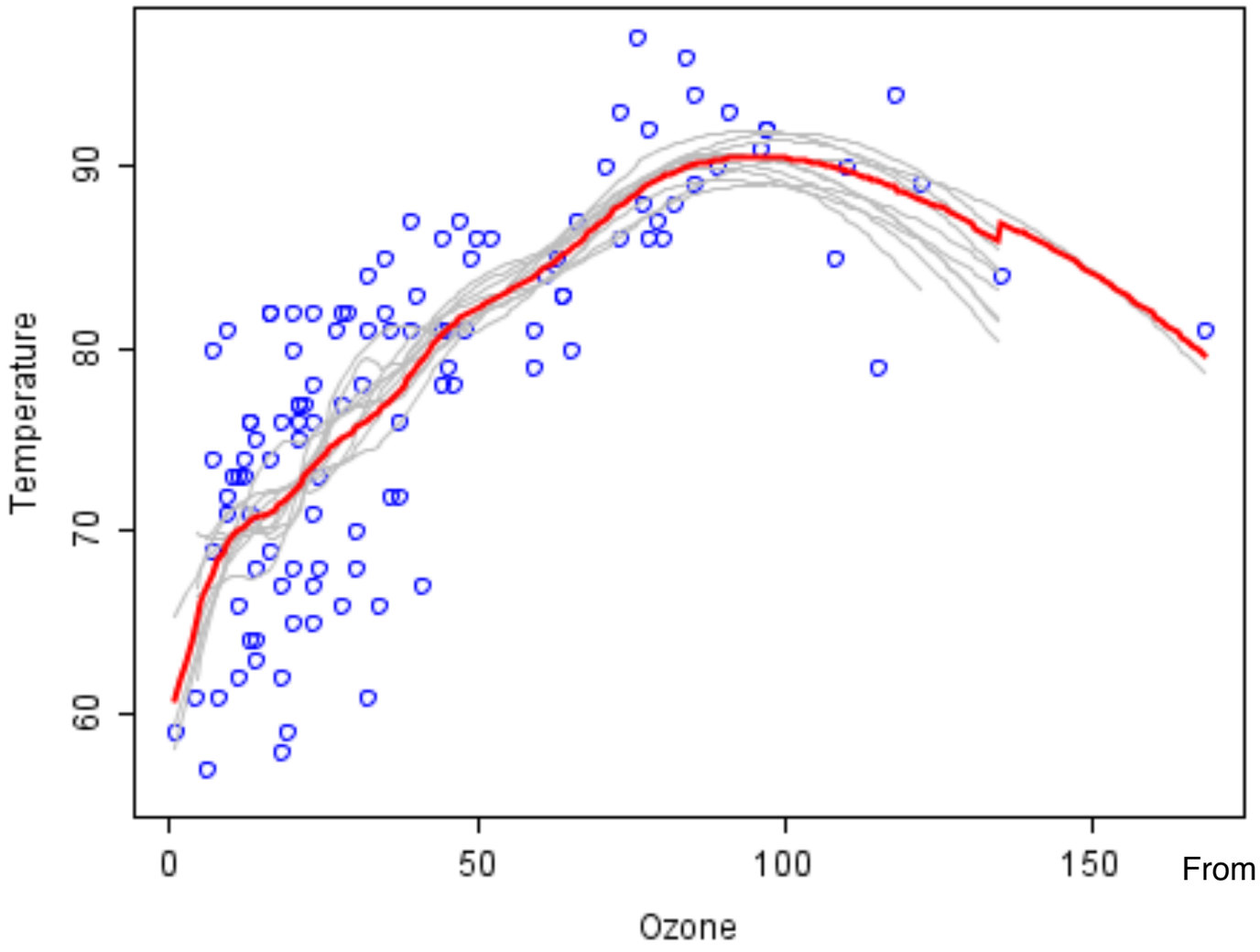
Similar properties as Jackknife.

Bagging

Bootstrap aggregating (Breiman, 1996): use Bootstrap to reduce the variance of predictions

- Construct Bootstrap samples $\mathcal{X}_i$, $|\mathcal{X}_i| = N$, $i \in \{1, \ldots, M\}$
- Train any model of choice on M datasets
- For a given test data point $\boldsymbol{x}$, obtain M predictions.
- Aggregate predictions
  - Regression: average
  - Classification: majority vote

Bagging



From Wikipedia

Random Subspace Method

- Problem with Bagging: datasets $\mathcal{X}_i$ are highly overlapping (~63%).
- Decision trees trained on $\mathcal{X}_i$ and their predictions become correlated.

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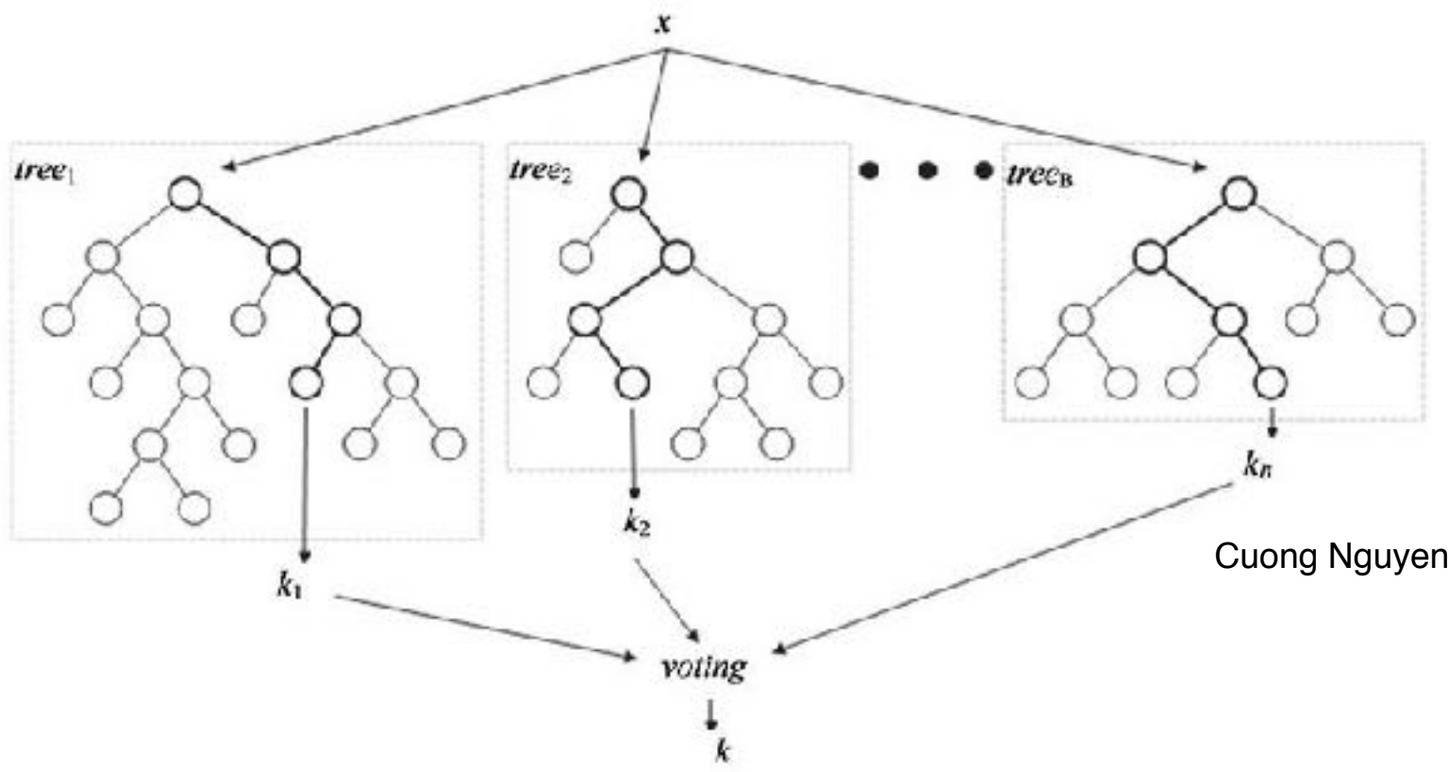
Random subspace method: construct new datasets by randomly sampling $d_B \leq d$ features without replacement. (Tin Kam Ho, 1998)

→ De-correlates estimators and decreases variance of the aggregate.

Random Forests

Combination of Bagging and random subspace method applied to decision trees. (Breiman, 1999)

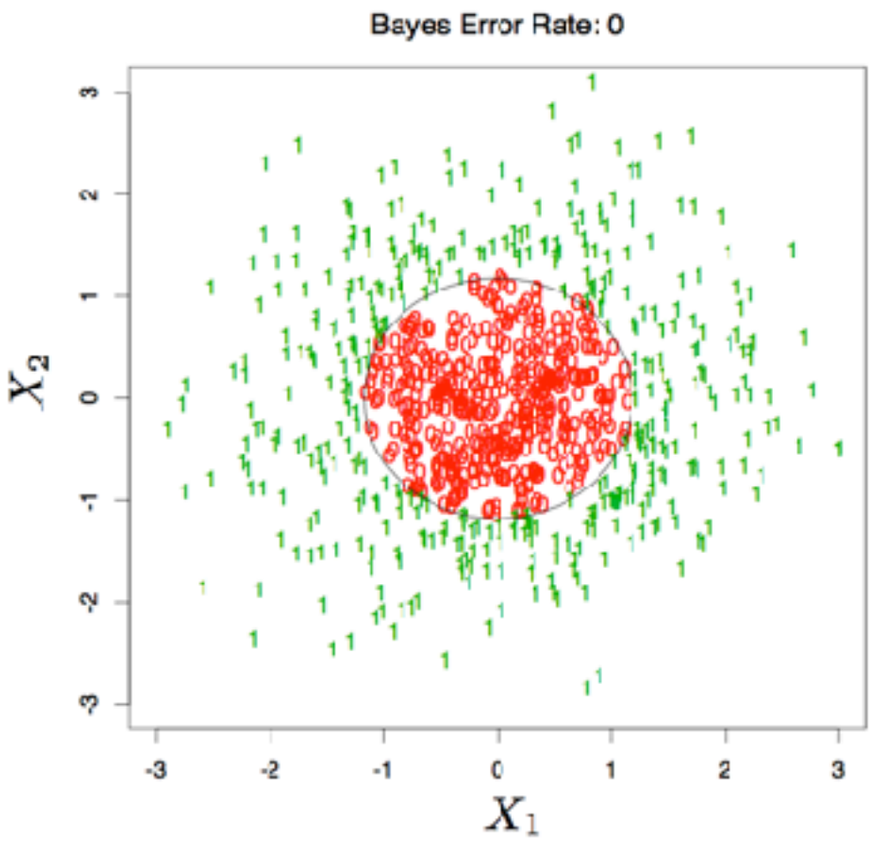
- Complexity control through out of bag monitoring.
- Random feature selection either at tree or split level.



Cuong Nguyen

Toy example

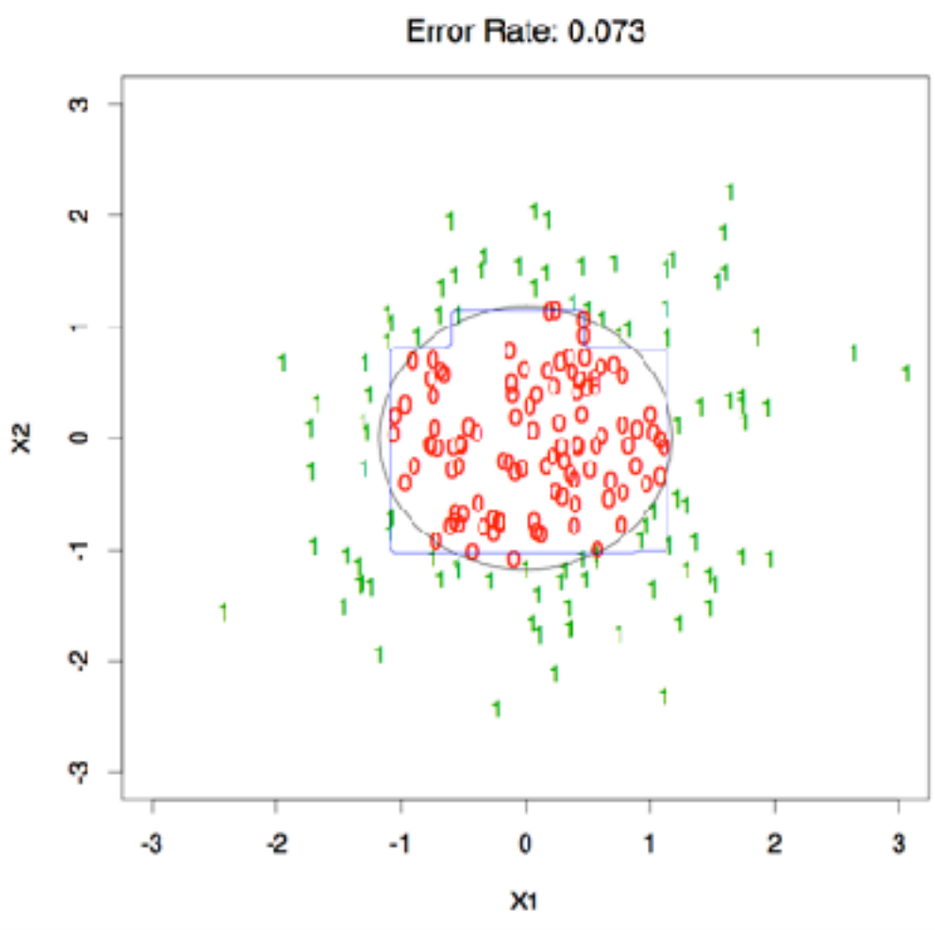
Toy Example - No Noise



- Deterministic problem; noise comes from sampling distribution of X.
- Use a training sample of size 200.
- Here Bayes Error is 0%.

Toy example

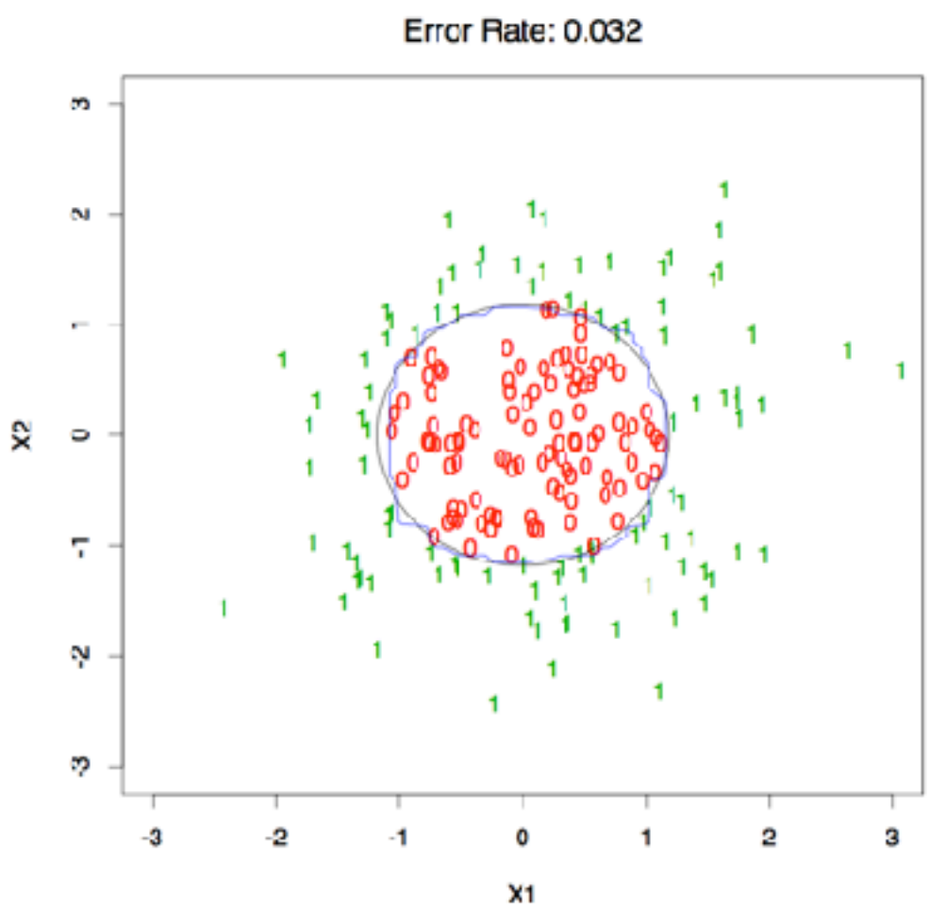
Decision Boundary: Tree



When the nested spheres are in 10-dimensions, Classification Trees produces a rather noisy and inaccurate rule $\hat{C}(X)$, with error rates around 30%.

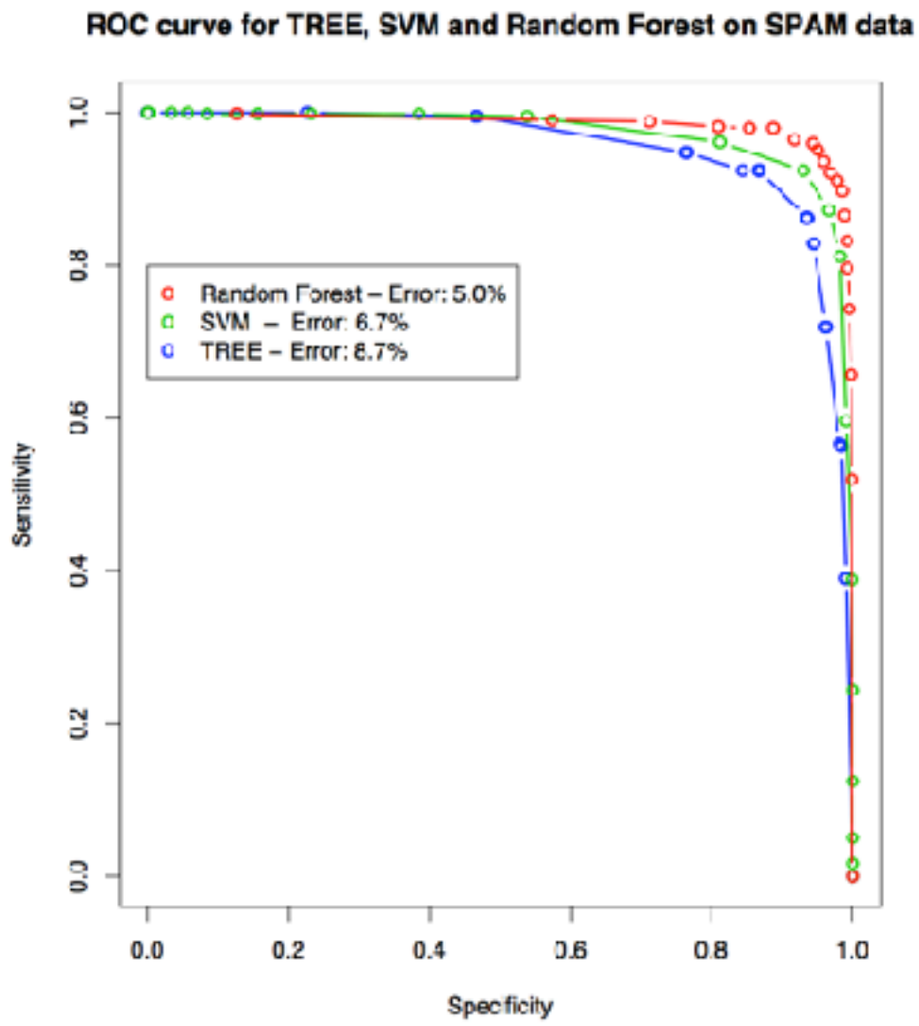
Toy example

Decision Boundary: Bagging



Bagging averages many trees, and produces smoother decision boundaries.

Toy example



TREE, SVM and RF

Random Forest dominates both other methods on the SPAM data — 5.0% error. Used 500 trees with default settings for `randomForest` package in `R`.

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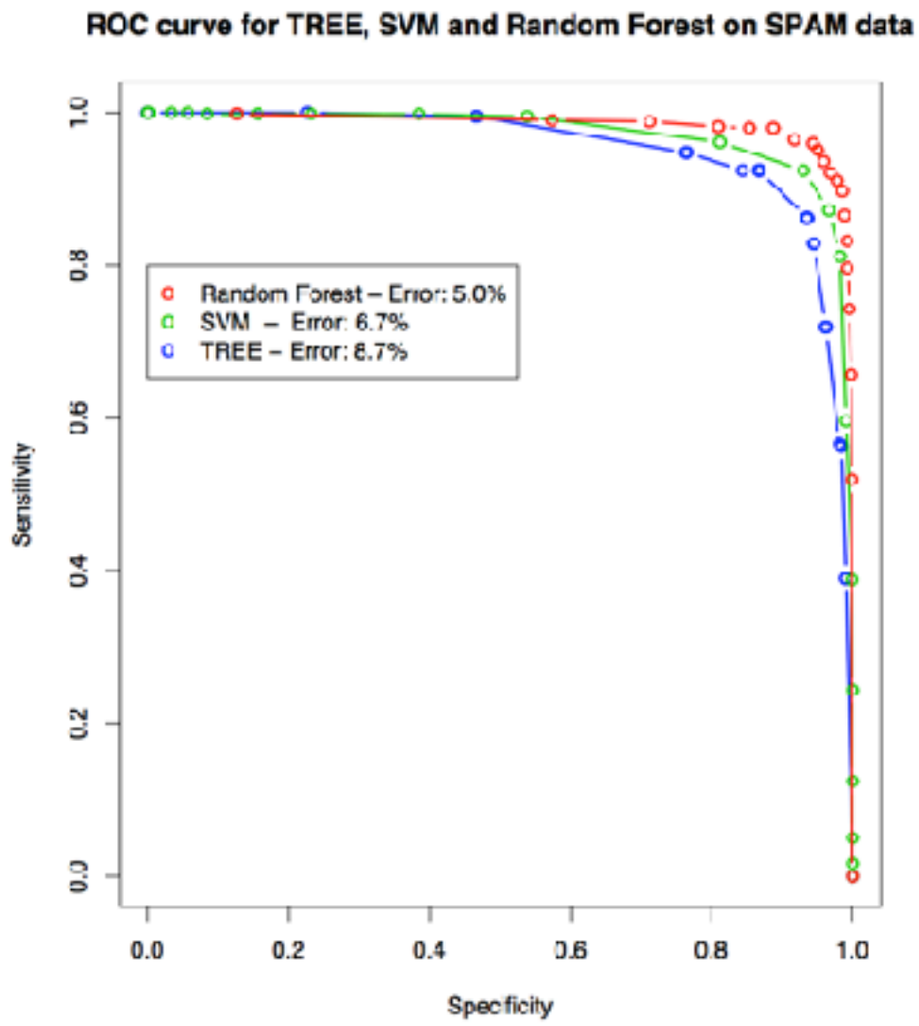

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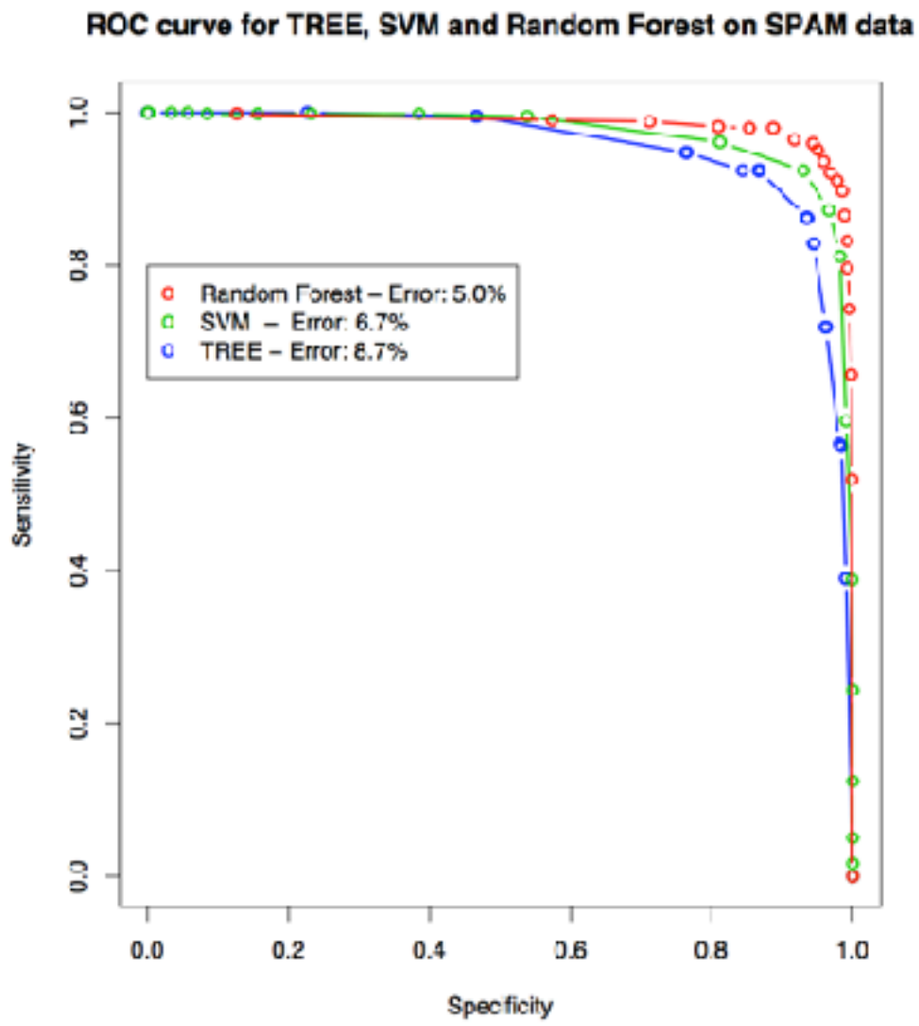

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Boosting

Consider the binary classification setting

$$\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^d \, ; y_1, \ldots, y_N \in \{+1, -1\}$$

A classifier, or 'hypothesis': $f(\mathbf{x}) : \mathbb{R}^d \mapsto \{+1, -1\}$, $f \in \mathcal{F}$

$\mathcal{F}$ is some hypothesis set (e.g. $f(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$)

Boosting

Consider the binary classification setting

$$\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^d \, ; y_1, \ldots, y_N \in \{+1, -1\}$$

A classifier, or 'hypothesis': $f(\mathbf{x}) : \mathbb{R}^d \mapsto \{+1, -1\}$, $f \in \mathcal{F}$

$\mathcal{F}$ is some hypothesis set (e.g. $f(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$)

0/1 classification loss: $l(f(x), y) = \begin{cases} 0 & \text{if } f(x) = y \\ 1 & \text{if } f(x) \neq y \end{cases}$

Empirical risk minimization: $R_{\text{emp}}(f) = \frac{1}{N} \sum_{i=1}^{N} l(f(\mathbf{x}_i), y_i)$

Boosting

Weighted ensemble learning: weighted majority vote over M hypotheses.

$$f_{\text{Ens}}(\mathbf{x}) = \sum_{i=1}^{M} a_i f_i(\mathbf{x}) \ , \ \ a_i \geq 0$$

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Bagging:

- $a_i = {}^1/_M$
- f_i are obtained using Bootstrap samples.

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Bagging:

- $a_i = {}^1/_M$
- f_i are obtained using Bootstrap samples.

Boosting:

- f_i are obtained from all samples, weighted by importance (soft selection)
- Sample weights: $d_i \in [0, 1] \ , \ i \in \{1, \ldots, N\} \ , \ \sum_{i=1}^{N} d_i = 1$
- Sample and hypothesis weights adapted over iterations 1, …, M

Motivation

- Difficult to achieve single classifier with high accuracy.
- But easy to devise ‘weak learners’ with non-random performance.
- **Definition:** $\exists \gamma \in [0, 1] \; \forall \{d_i\} \; \forall \mathcal{X} \forall \mathcal{Y} \; \varepsilon(f, \mathbf{d}) < \frac{1}{2}(1 - \gamma)$,

  where $\varepsilon(f, \mathbf{d}) = \sum_{i=1}^{N} d_i l(f(\mathbf{x}_i), y_i)$ is the weighted training error.

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  where $\varepsilon(f, \mathbf{d}) = \sum_{i=1} d_i l(f(\mathbf{x}_i), y_i)$ is the weighted training error.
- **Idea:** combine the hypotheses of different weak learners.
- **In practice:** same algorithm trained on differently weighted samples.
- Iterate with higher emphasis (weight) on misclassified examples.
- **Final hypothesis:** sum of weak hypotheses, weighted by training acc.

Analogy: horse-racing bets

- Nobody is really good in predicting a horse race
- But everybody has some rule of thumb that is better than random (teeth, chest, history, jockey weight)
- Strategy: present learner with races that are hardest to predict according to current model

→ ‘Maximal information gain’ per expert consultation

AdaBoost

Algorithm 1 (Discrete) AdaBoost (Freund and Schapire, 1996)

Input: sample $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$, number of iterations M

Initialize: $d_i^{(1)} = \frac{1}{N}$, $i = 1, \ldots, N$

1: **for** $m = 1, \ldots, M$ **do**

2: Train classifier on weighted sample $\left\{(d_1^{(t)}, \mathbf{x}_1, y_1), \ldots, (d_N^{(t)}, \mathbf{x}_N, y_N)\right\}$ and obtain hypothesis $f^{(m)}(\mathbf{x})$

3: Calculate weighted training error: $\varepsilon^{(m)} = \sum_{i=1}^{N} d_i^{(t)} I(f^{(m)}(\mathbf{x}_i), y_i)$

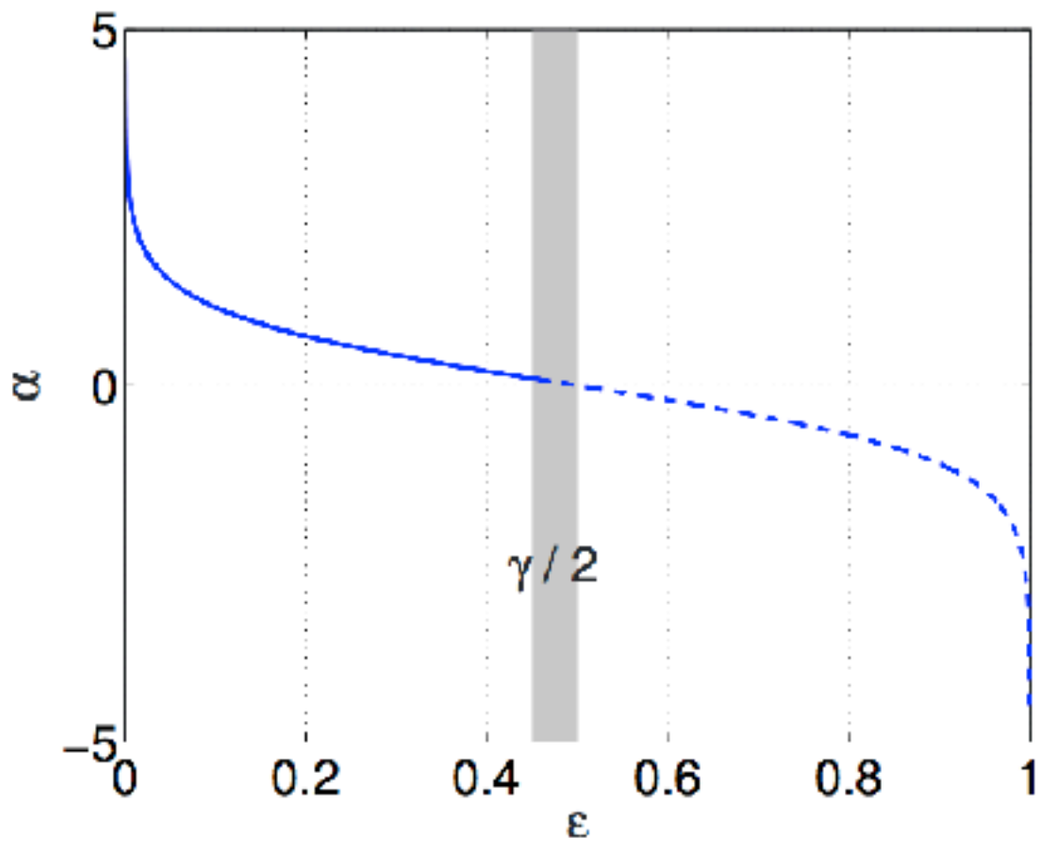
4: Assign weight to $f^{(m)}$: $\alpha^{(m)} = \frac{1}{2} \ln \frac{1-\varepsilon^{(m)}}{\varepsilon^{(m)}}$

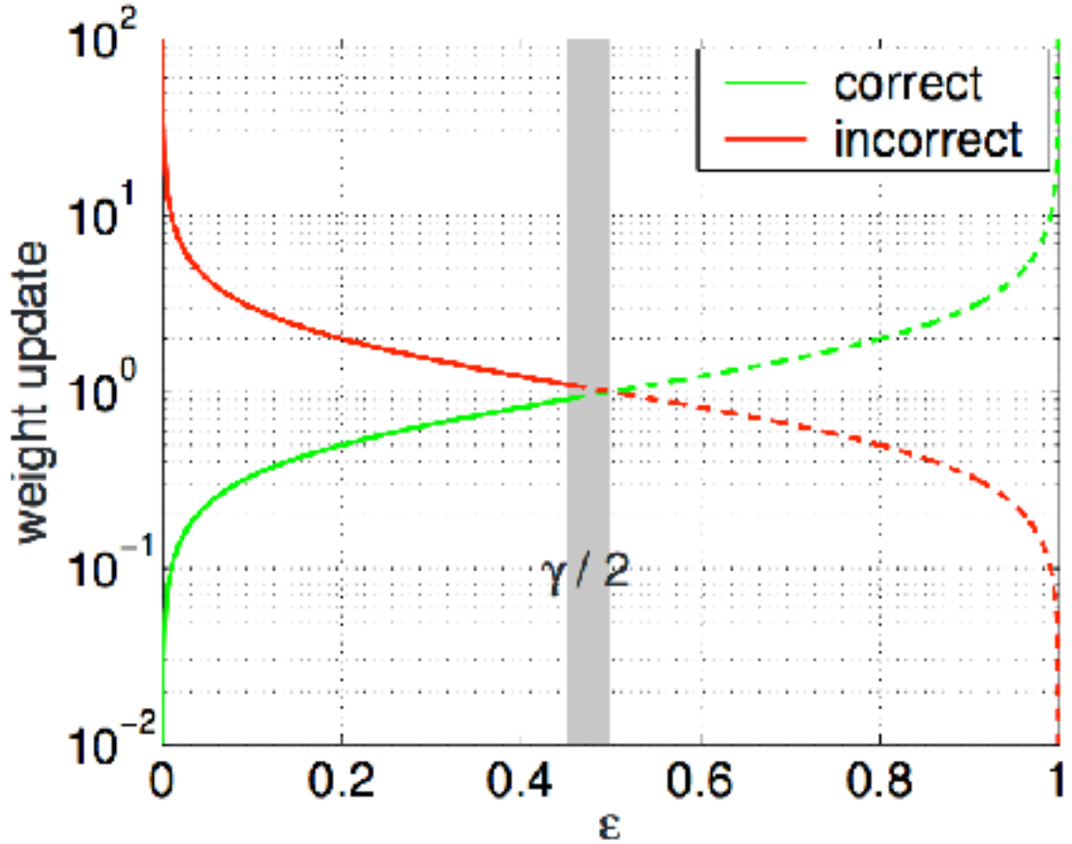
5: Update sample weights: $d_i^{(m+1)} = d_i^{(m)} \exp(-\alpha_m y_i f^{(m)}(\mathbf{x}_i))/Z^{(m)}$,
$Z^{(m)} = \sum_{i=1}^{N} d_i^{(m)} \exp(-\alpha_m y_i f^{(m)}(\mathbf{x}_i))$

6: **end for**

Final hypothesis: $f(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m f^{(m)}(\mathbf{x})\right)$

AdaBoost: weights





AdaBoost

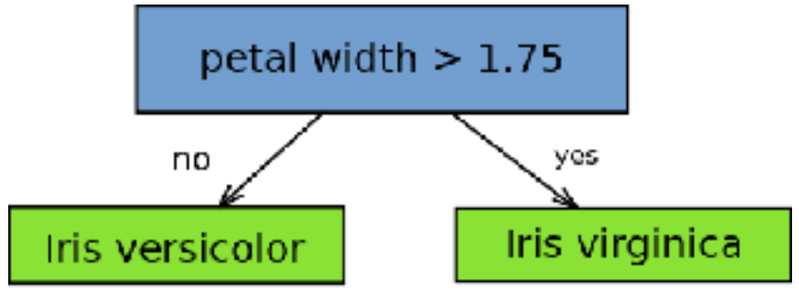
Choices of weak learners

- Trees

AdaBoost

Choices of weak learners

- Trees
- Stumps



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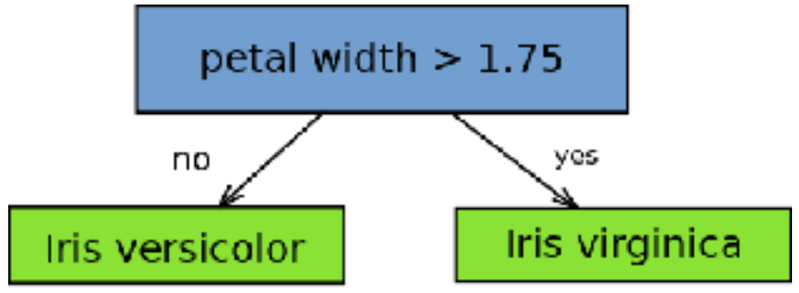

How to train on a weighted sample?

- Incorporate d in the loss function of the classifier.

e.g. $\min_{w,\xi,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N} p_i \xi_i \quad \text{s.t. } \forall i \ : \ y_i(w^\top x_i + b) \geq 1 - \xi_i, \ \ \xi_i \geq 0.$

AdaBoost

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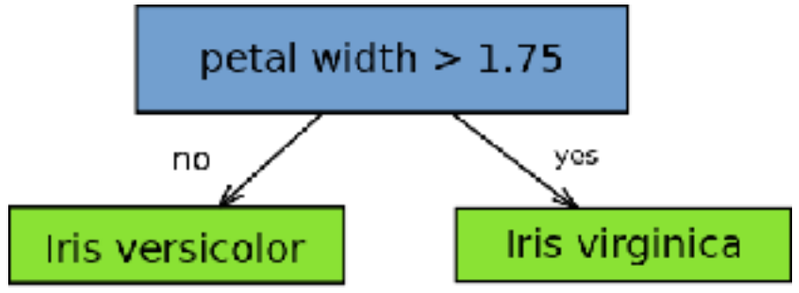

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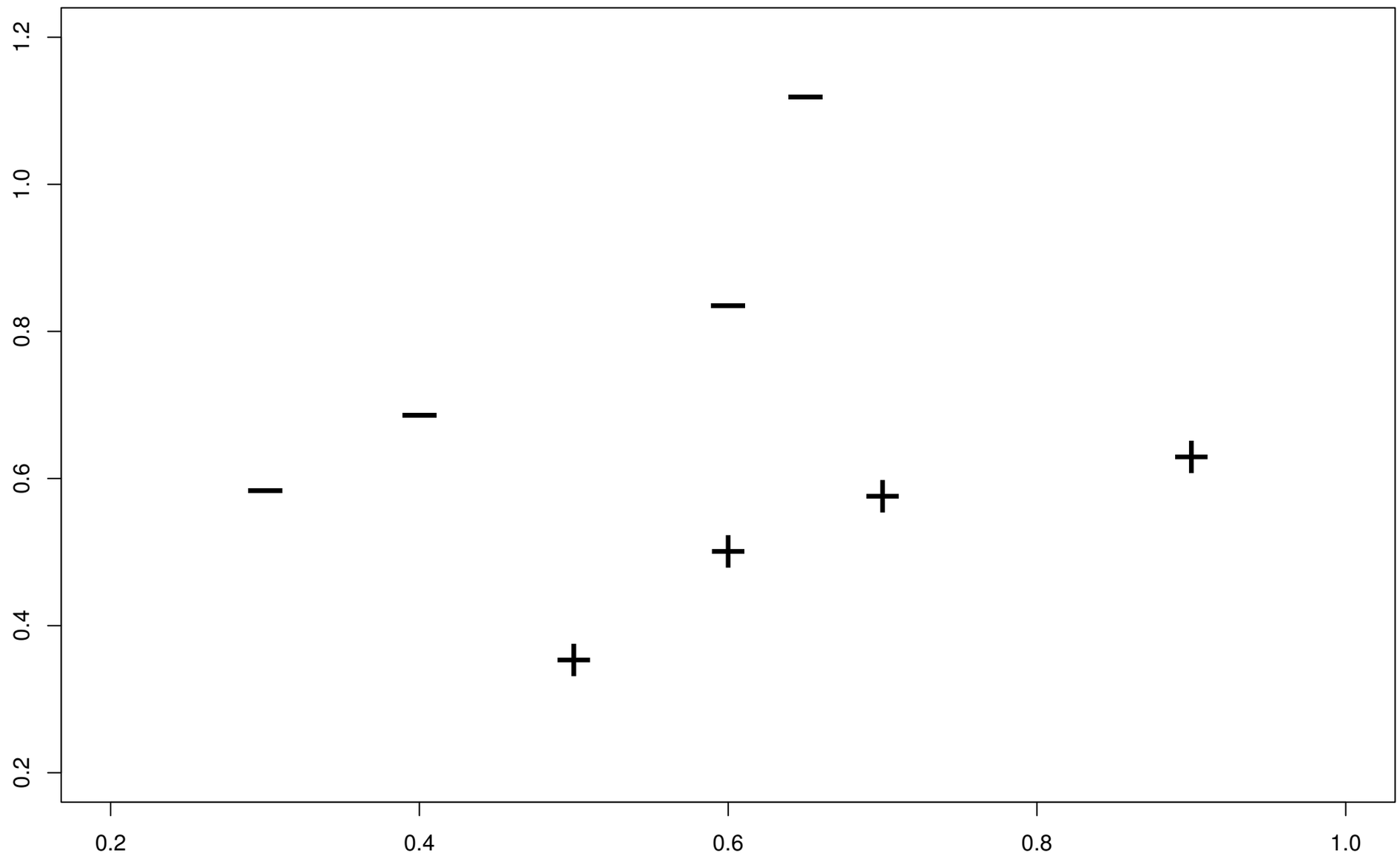
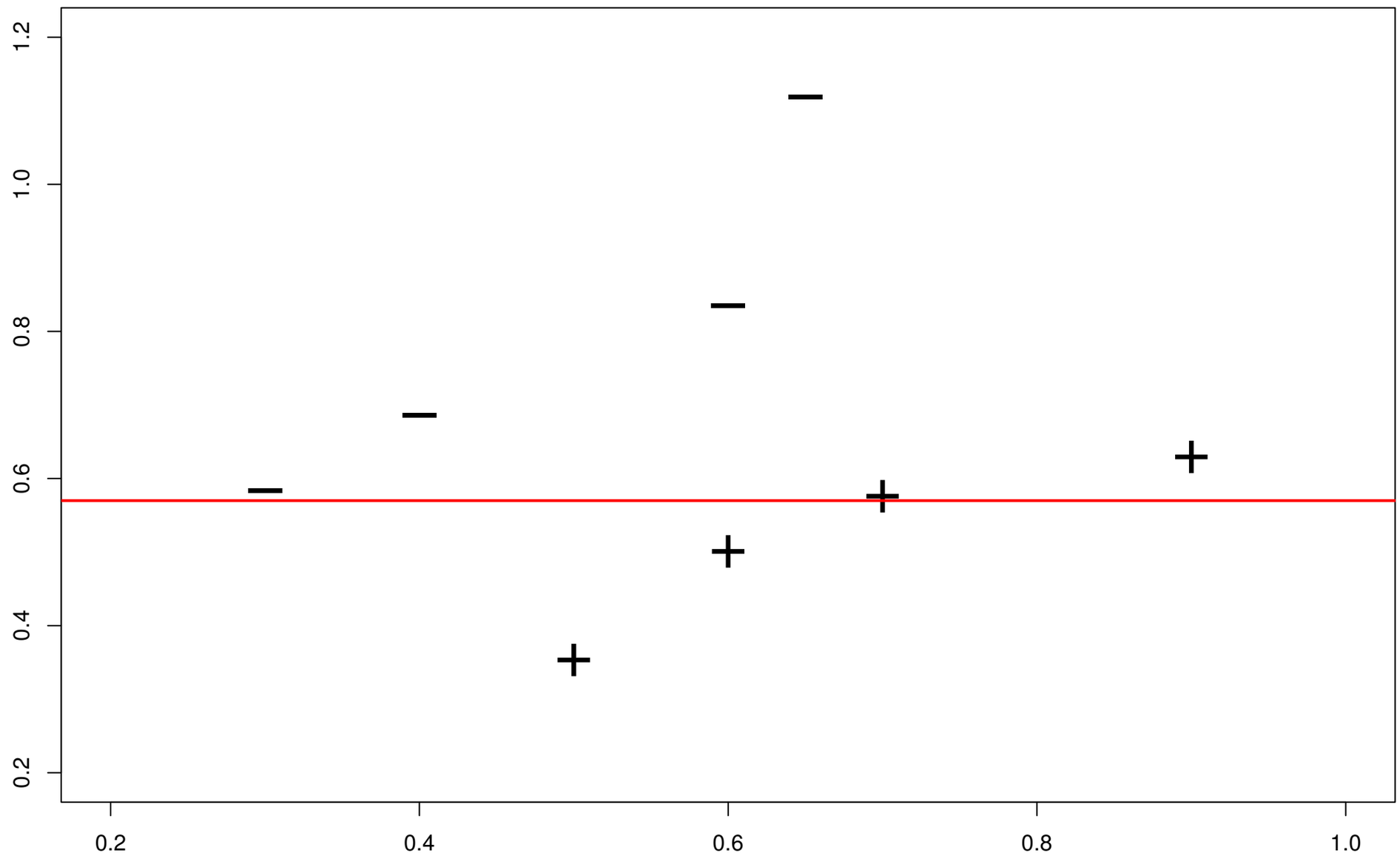
- Over-sample data to follow ‘distribution’ d.

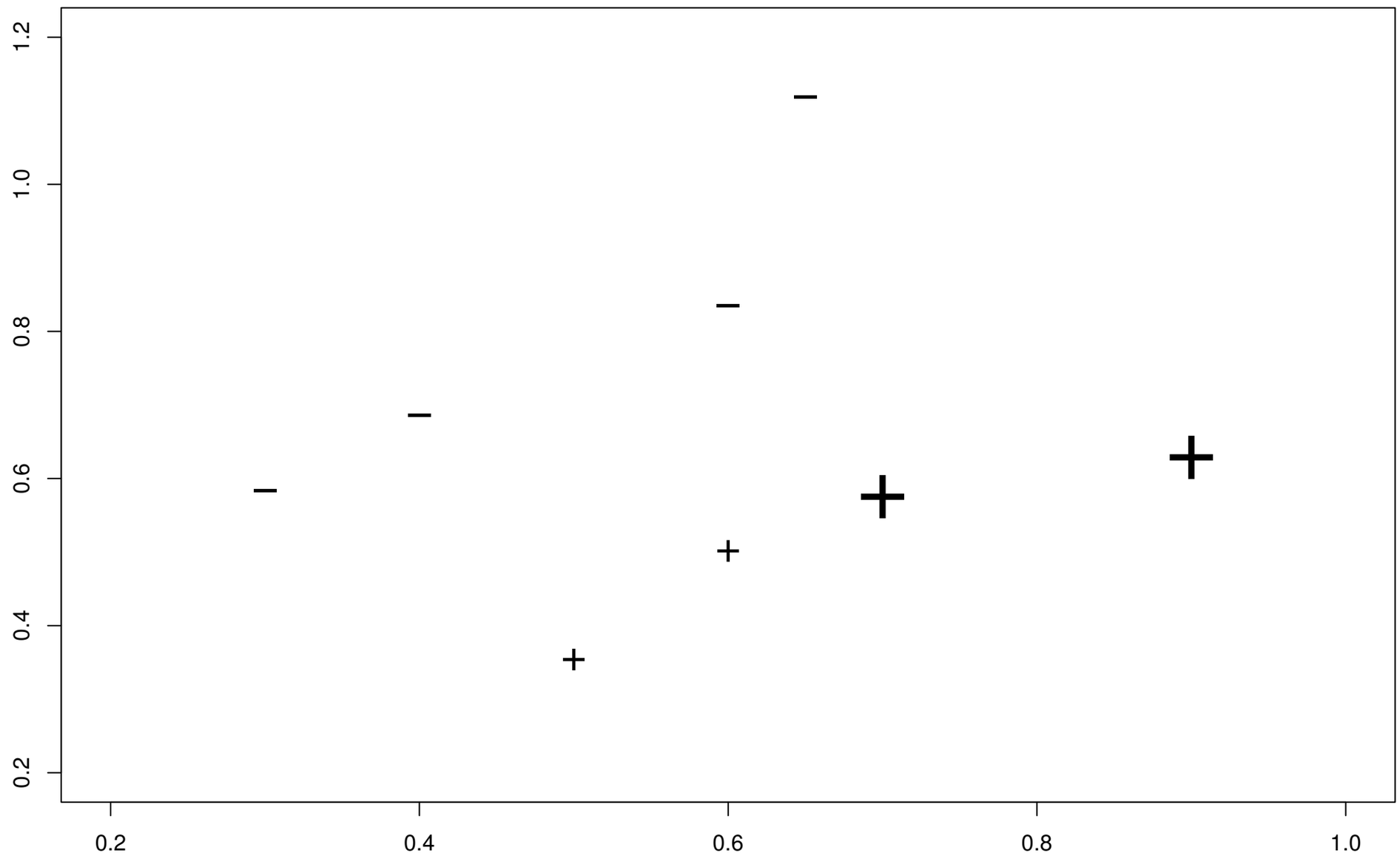
Example



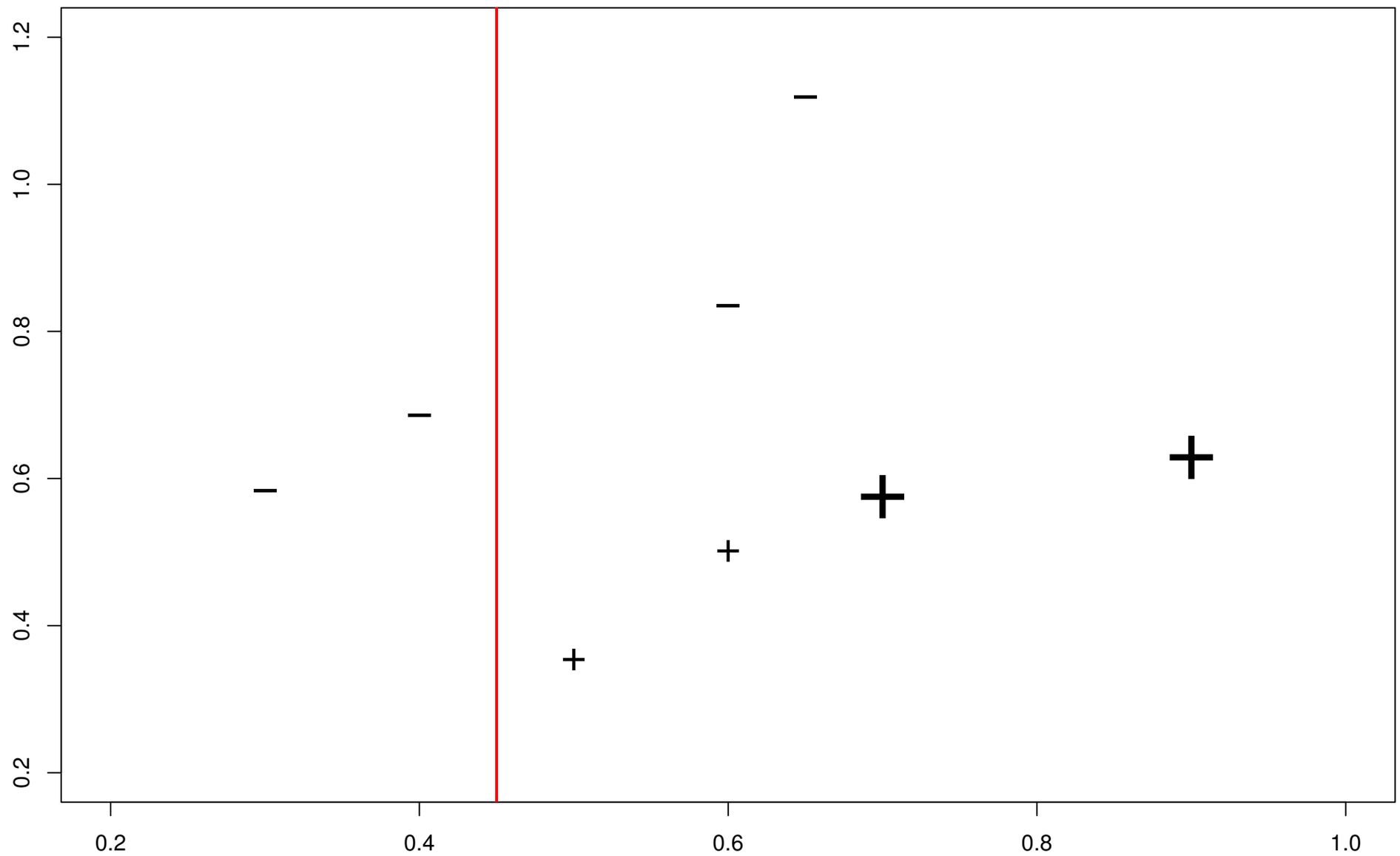
Example



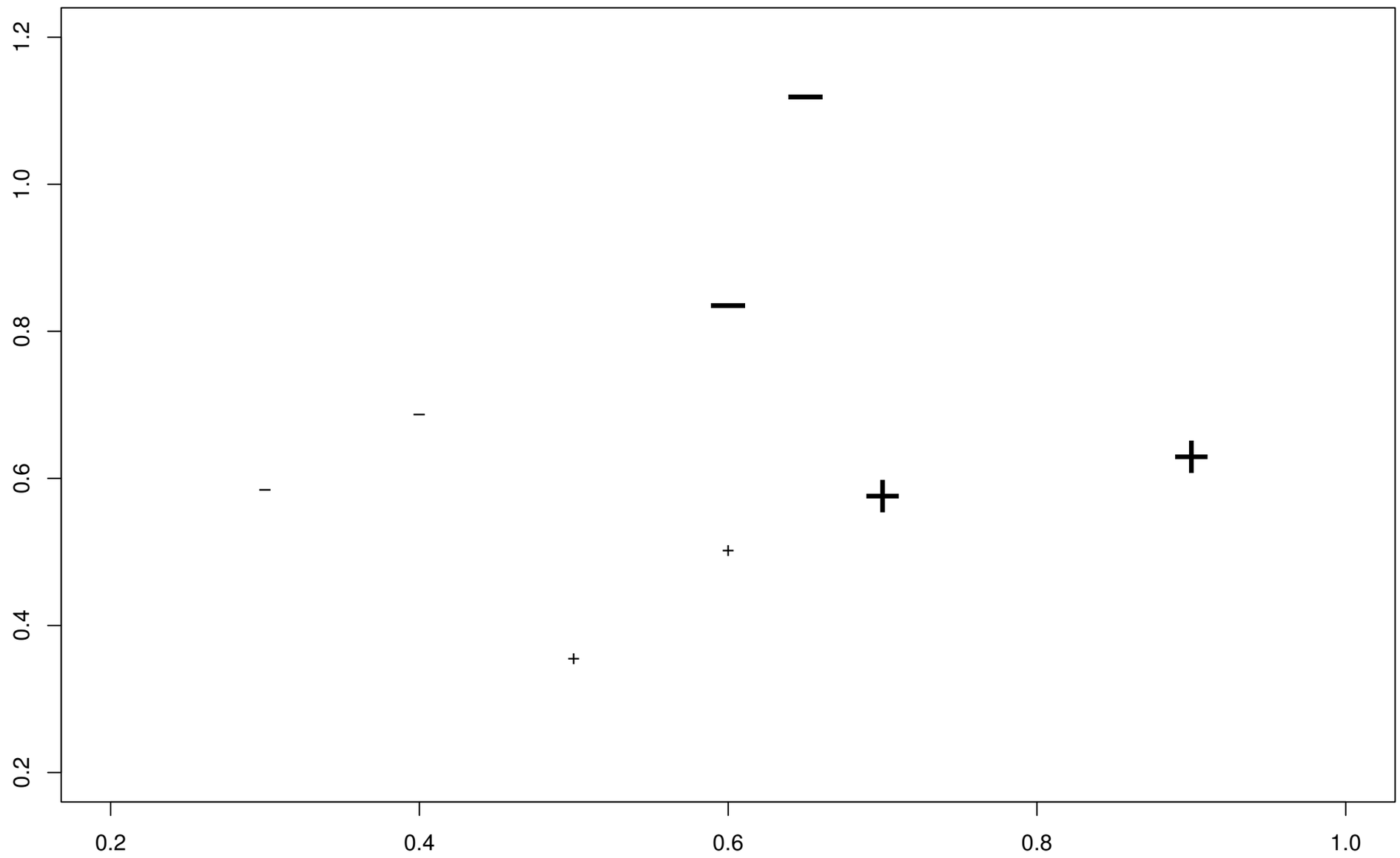
Example



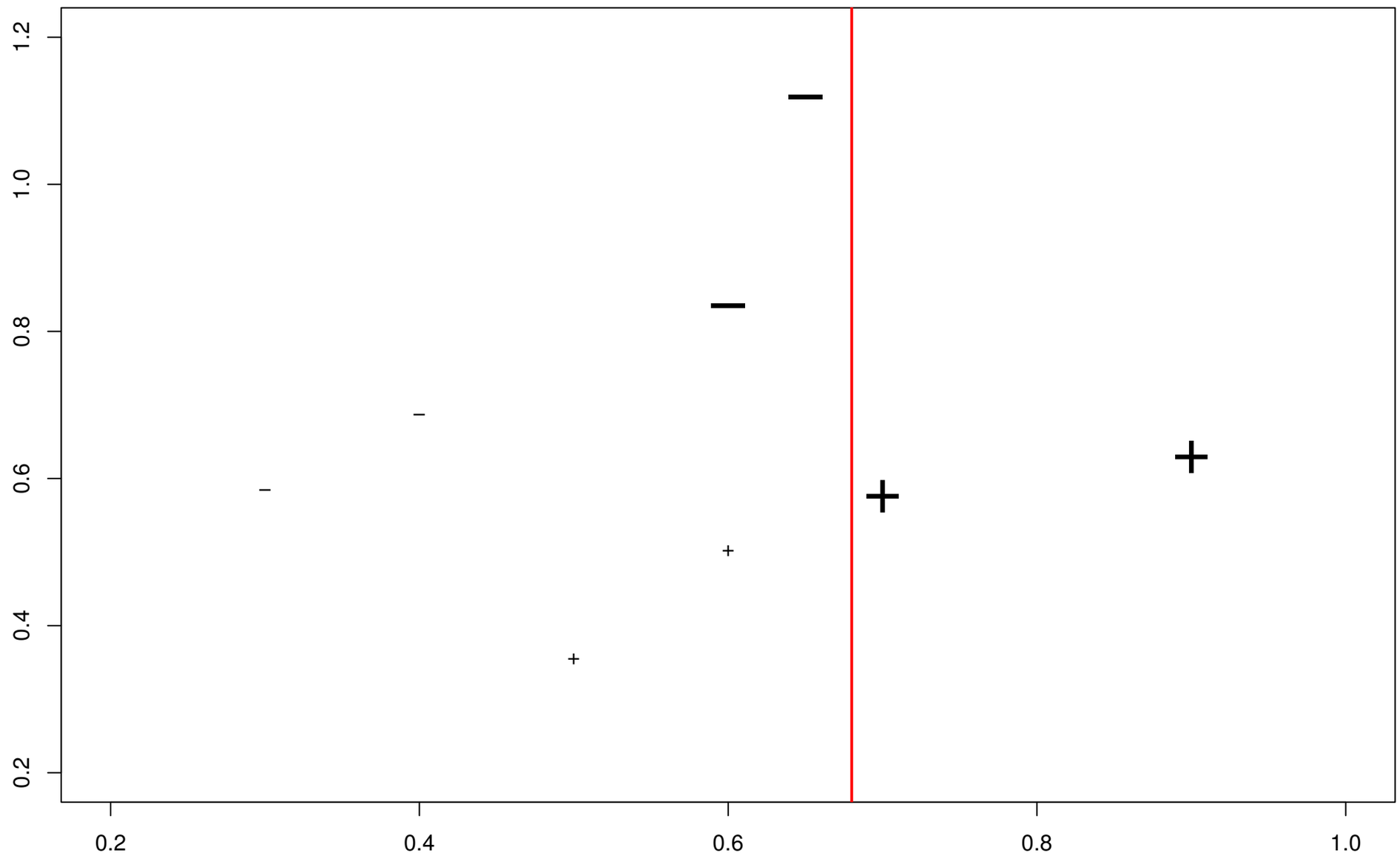
Example



Example



Example



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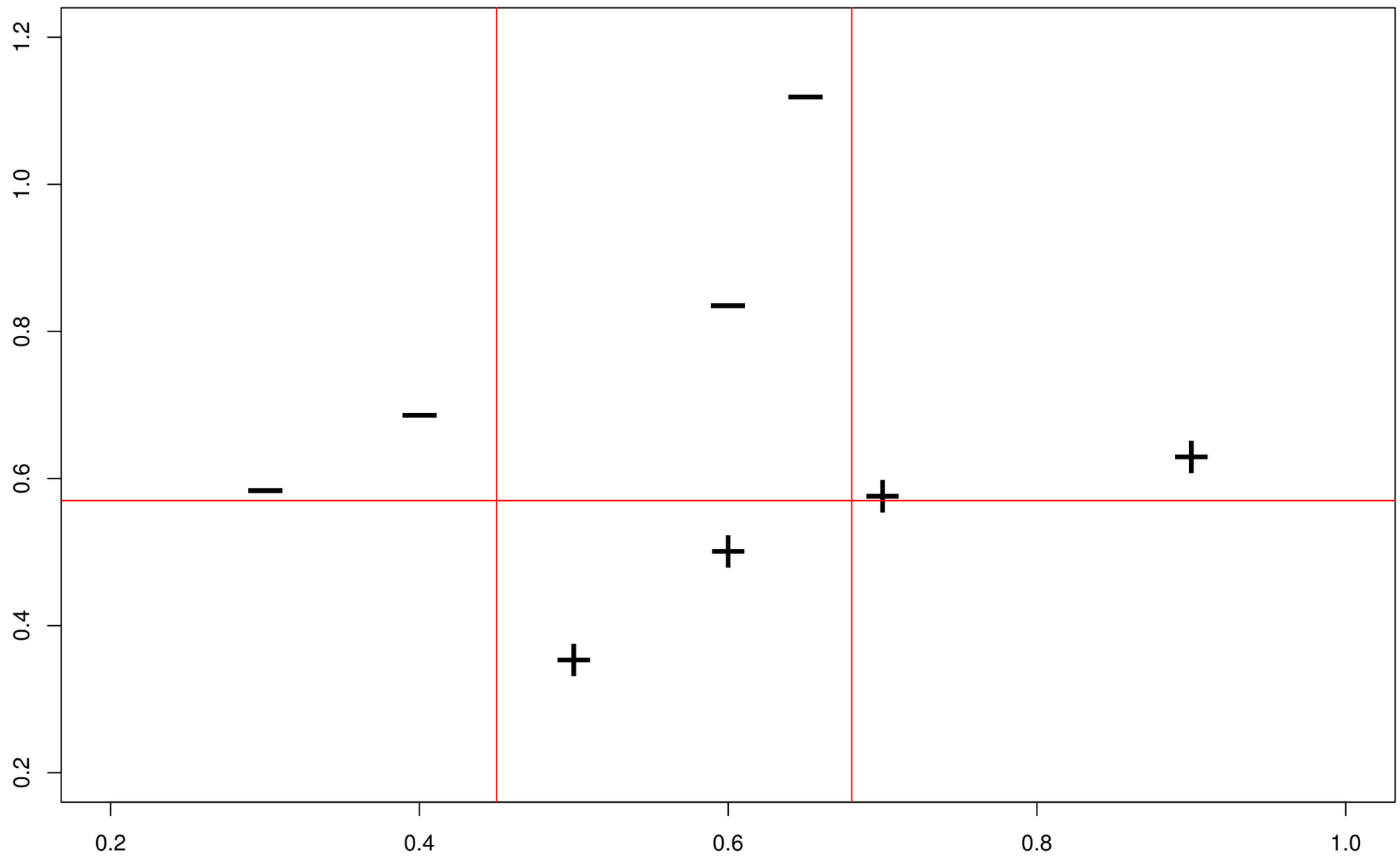

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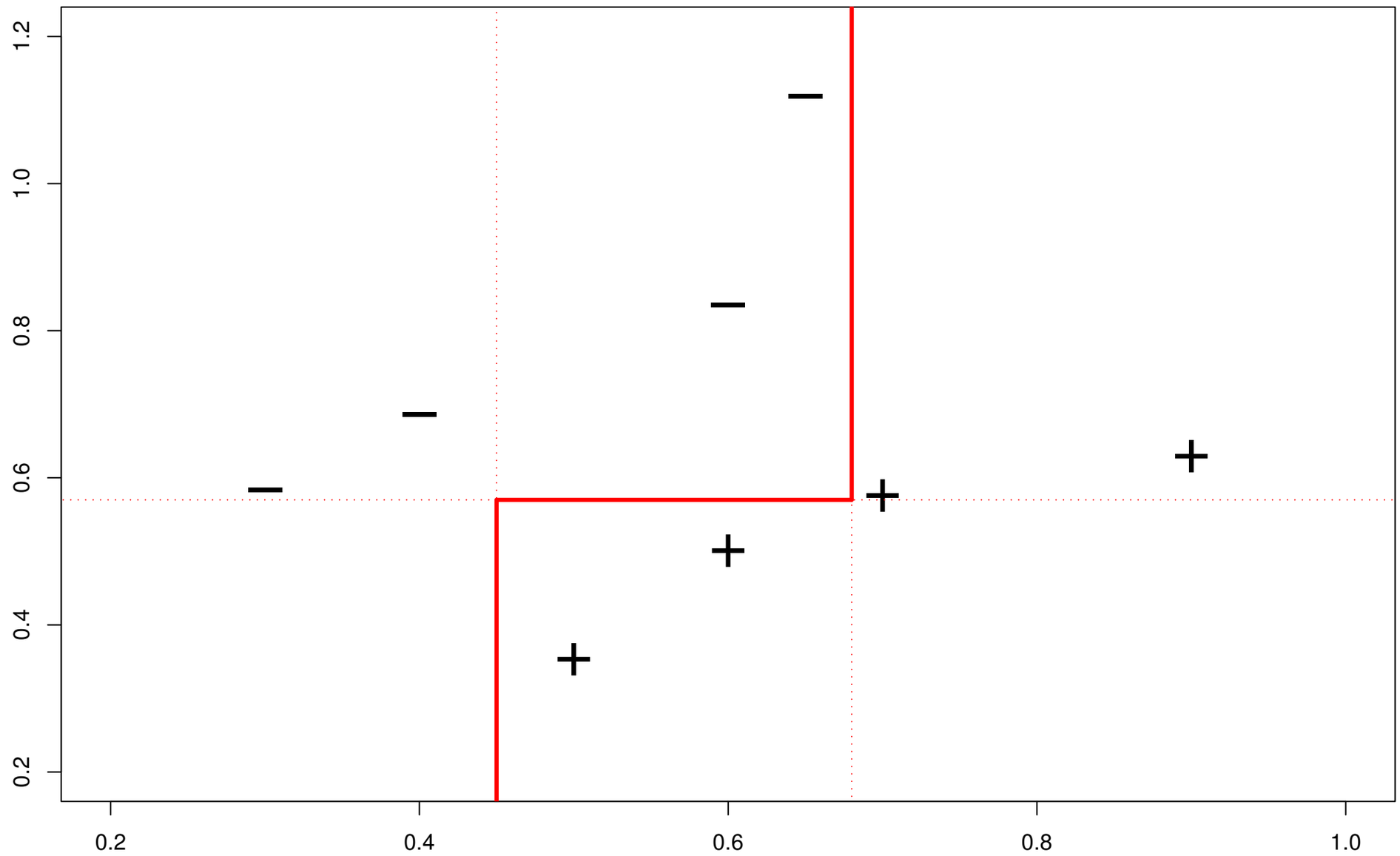
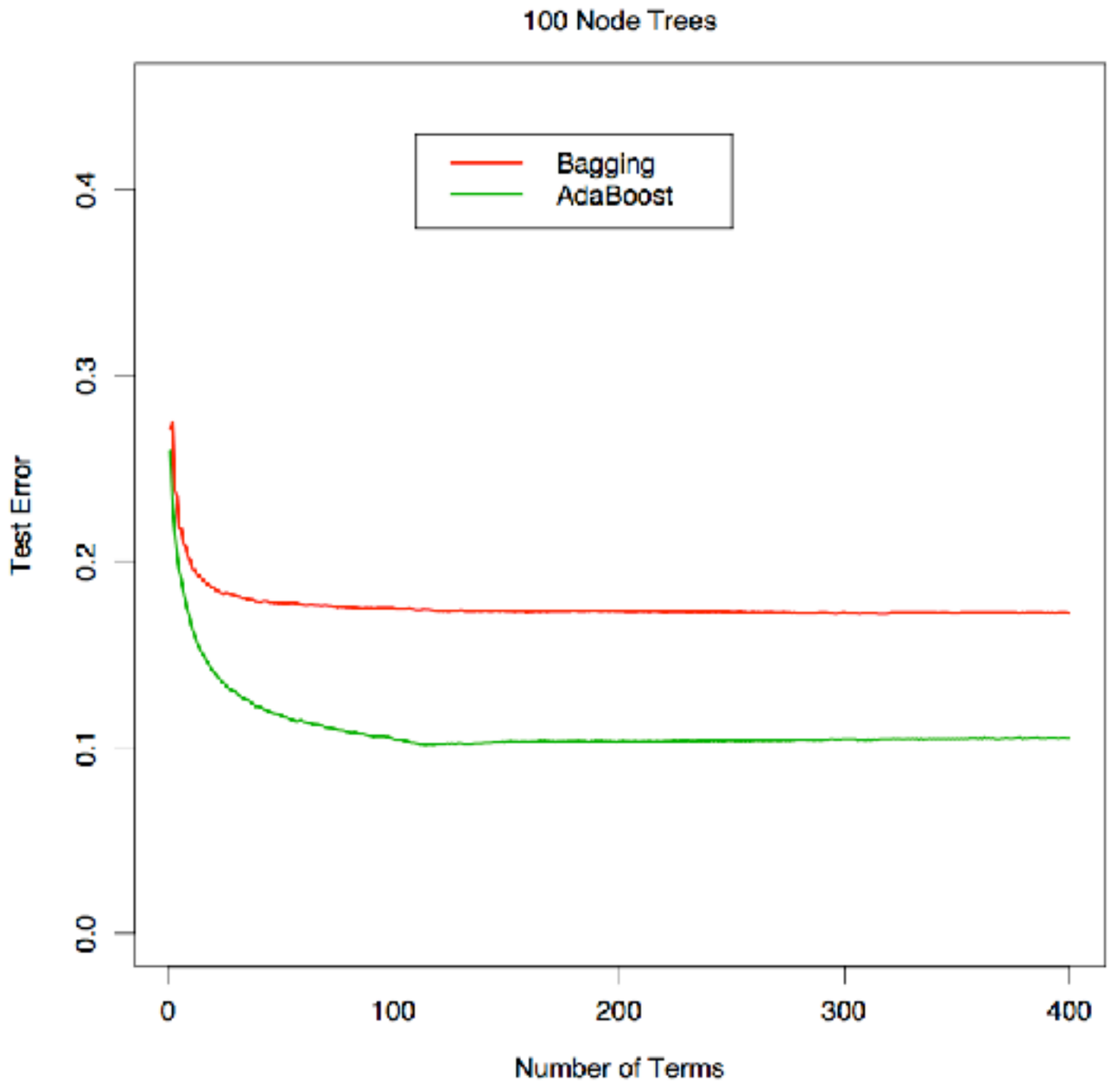


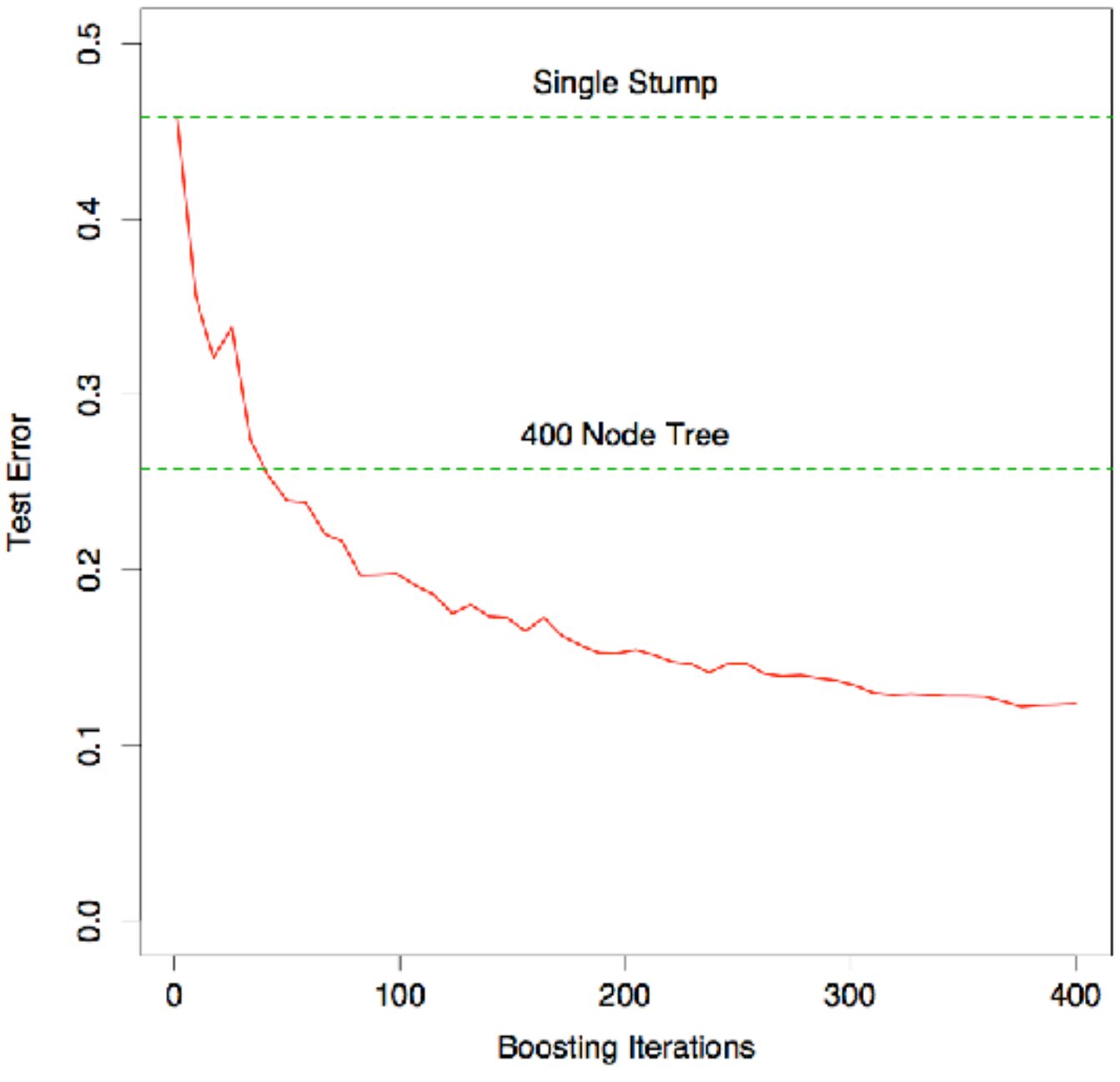
Toy example revisited



Boosting vs Bagging

- 2000 points from Nested Spheres in R^{10}
- Bayes error rate is 0%.
- Trees are grown best first without pruning.
- Leftmost term is a single tree.

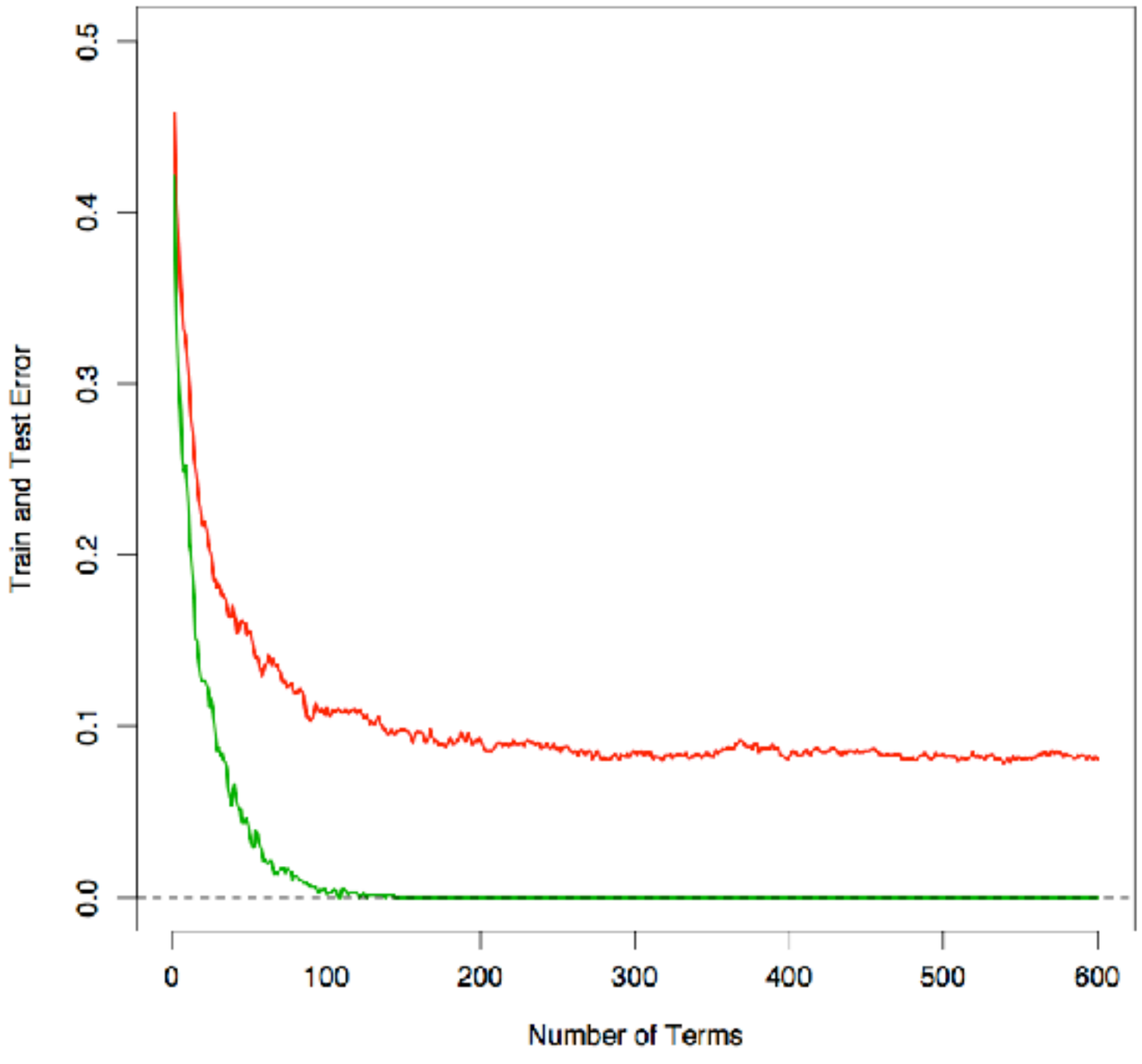
Toy example revisited



Boosting Stumps

A stump is a two-node tree, after a single split. Boosting stumps works remarkably well on the nested-spheres problem.

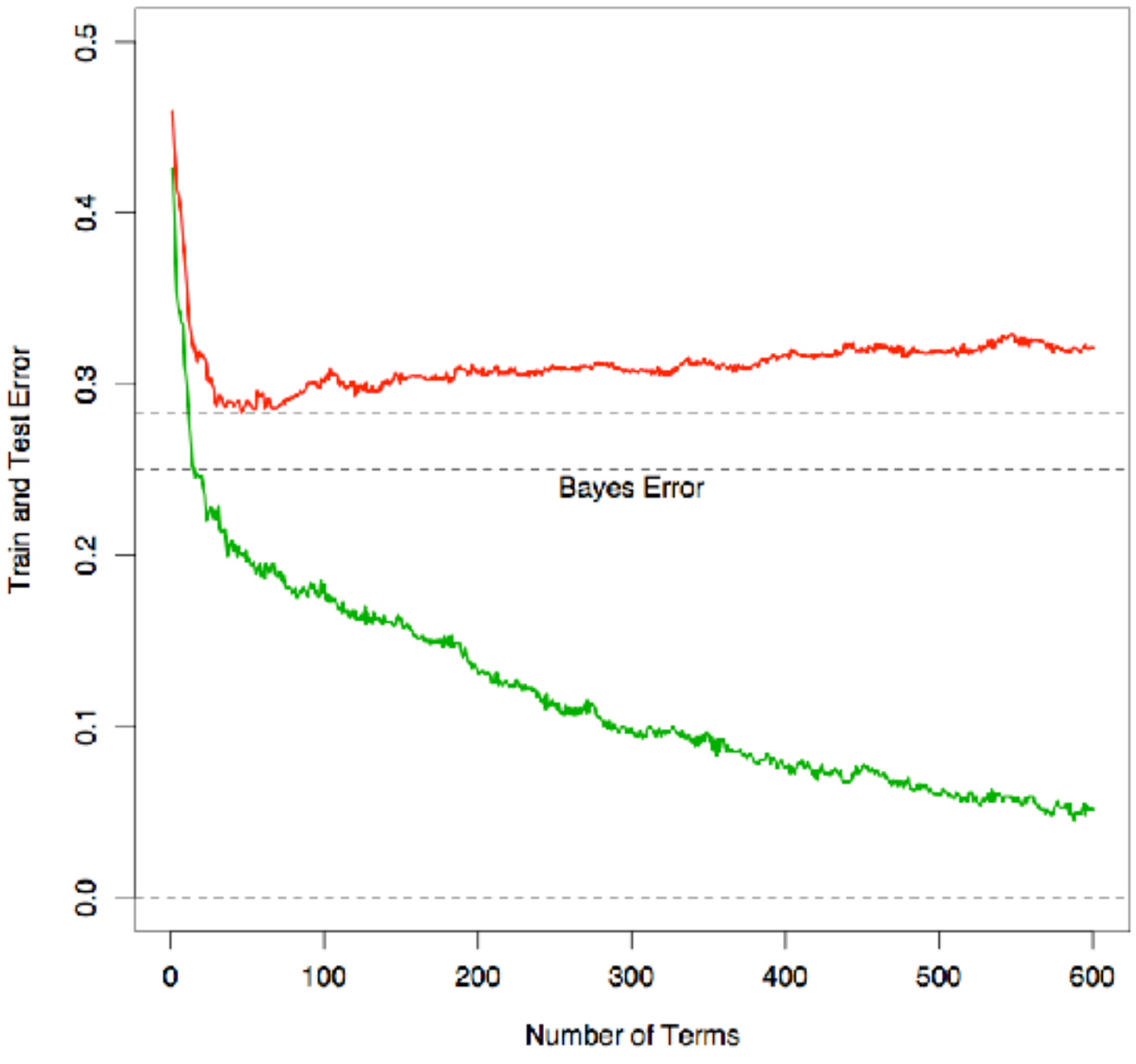
Toy example revisited



Training Error

- Nested spheres in 10-Dimensions.
- Bayes error is 0%.
- Boosting drives the training error to zero.
- Further iterations continue to improve test error in many examples.

Toy example revisited



Noisy Problems

- Nested Gaussians in 10-Dimensions.
- Bayes error is 25%.
- Boosting with stumps
- Here the test error does increase, but quite slowly.

Boosting as gradient descent

- AdaBoost stepwise minimizes a function of $y_i f_{\boldsymbol{\alpha}}(x_i) = y_i \sum_t \alpha_t h_t(\mathbf{x}_i)$

$$\mathcal{G}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\}$$

- The gradient of $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ gives exactly the example weights used for AdaBoost:

$$\frac{\partial \mathcal{G}(\boldsymbol{\alpha}^{(t)})}{\partial f(\mathbf{x}_i)} \sim \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\} \sim d_i^{(t+1)}$$

- The hypothesis coefficient α_t is chosen, such that $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ is minimized:

$$\alpha_t = \underset{\alpha_t \geq 0}{\operatorname{argmin}}\, \mathcal{G}(\boldsymbol{\alpha}^{(t)}) = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$$

- **AdaBoost is a gradient descent method to minimizes $\mathcal{G}(\boldsymbol{\alpha})$.**

Convergence

Theorem 1 (Schapire et al. 1997) *Suppose AdaBoost generates hypotheses with weighted training errors* $\epsilon_1, \ldots, \epsilon_T$. *Then we have*

$$\sum_{i=1}^{N} \mathrm{I}(y_i \neq \mathrm{sign}(f_{Ens}(\mathbf{x}_i))) \leq 2^T \prod_{t=1}^{T} \sqrt{\epsilon_t(1-\epsilon_t)}$$

If $\epsilon_t < \frac{1}{2} - \frac{1}{2}\gamma$ (for all $t = 1, \ldots, T$), then the training error will decrease exponentially fast, i.e. will be **zero** after only

$$\frac{2\log(N)}{\gamma^2} = \mathcal{O}(\log(N))$$

iterations.

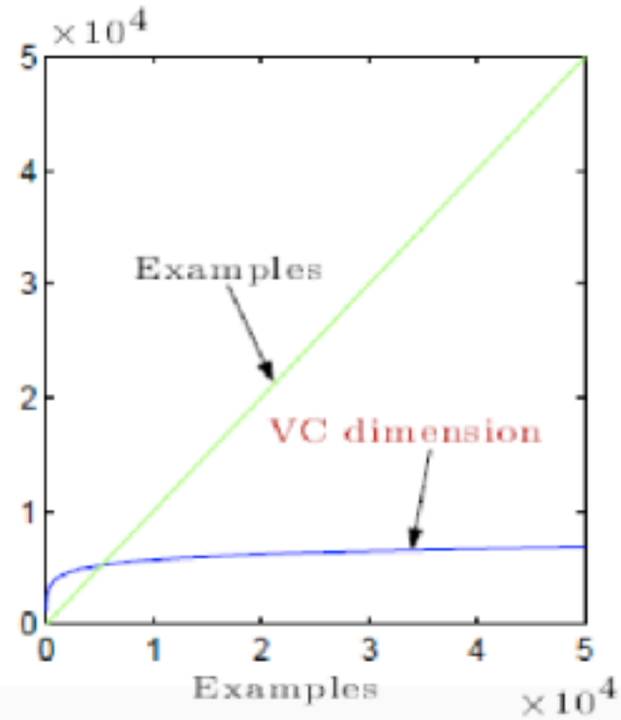
VC dimension

Let d be the VC dimension of the base hypothesis class $\mathcal{H}$.
Then the VC dimension of the class of combined functions is

$$d_{Ens}(N, \gamma) = \mathcal{O}\Big(d \underbrace{\frac{\log(N)}{\gamma^2}}_{\sim T} \log\left(\frac{\log(N)}{\gamma^2}\right)\Big) = \mathcal{O}\left(d \log(N) \log^2(N)\right).$$

An Example

- VC dimension $d = 2$
  (e.g. decision stumps)
- $\epsilon_t \leq 0.4 = \frac{1}{2} - \frac{1}{2}\gamma$
  $\Rightarrow \gamma \geq 0.2$



Theory

- properties of weak learner imply exponential convergence to a consistent hypothesis
- Fast convergence ensures small VC dimension of the combined hypothesis
- small VC implies small deviation from the empirical risk
- for any $\varepsilon > 0$ and $\delta > 0$ exists a sample size N, such that with probability $1 - \delta$ the expected risk is smaller than ε
- Any weak learner can be boosted to achieve an arbitrary high accuracy! ($\rightsquigarrow$ strong learner)

Similarities to SVM's

- AdaBoost maximizes the margin.
- Examples with stable large weights emerge during optimization

  → Support Vectors
- Formulation as a mathematical program similar to SVM possible

  → Regularized Boosting possible

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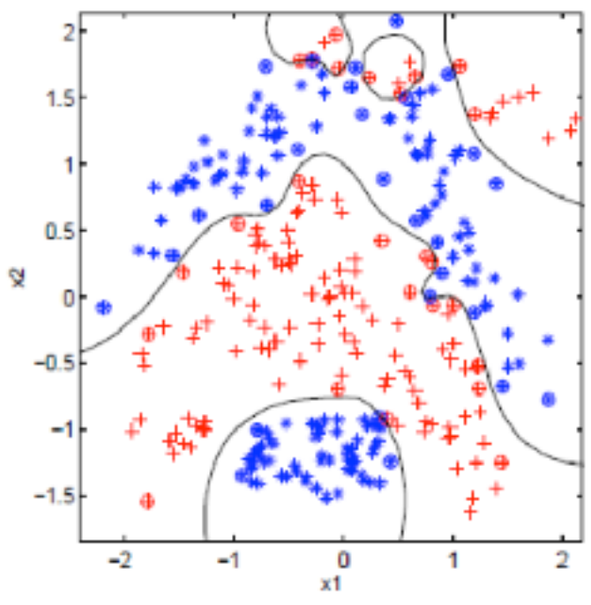
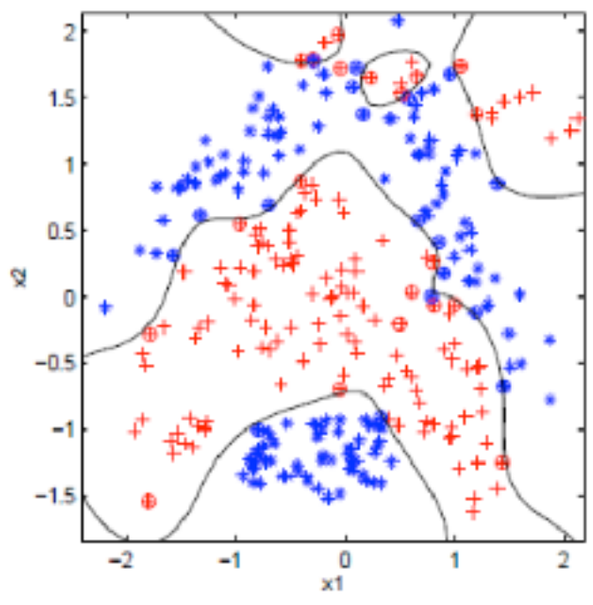


AdaBoost's decision line



SVM's decision line

Real data

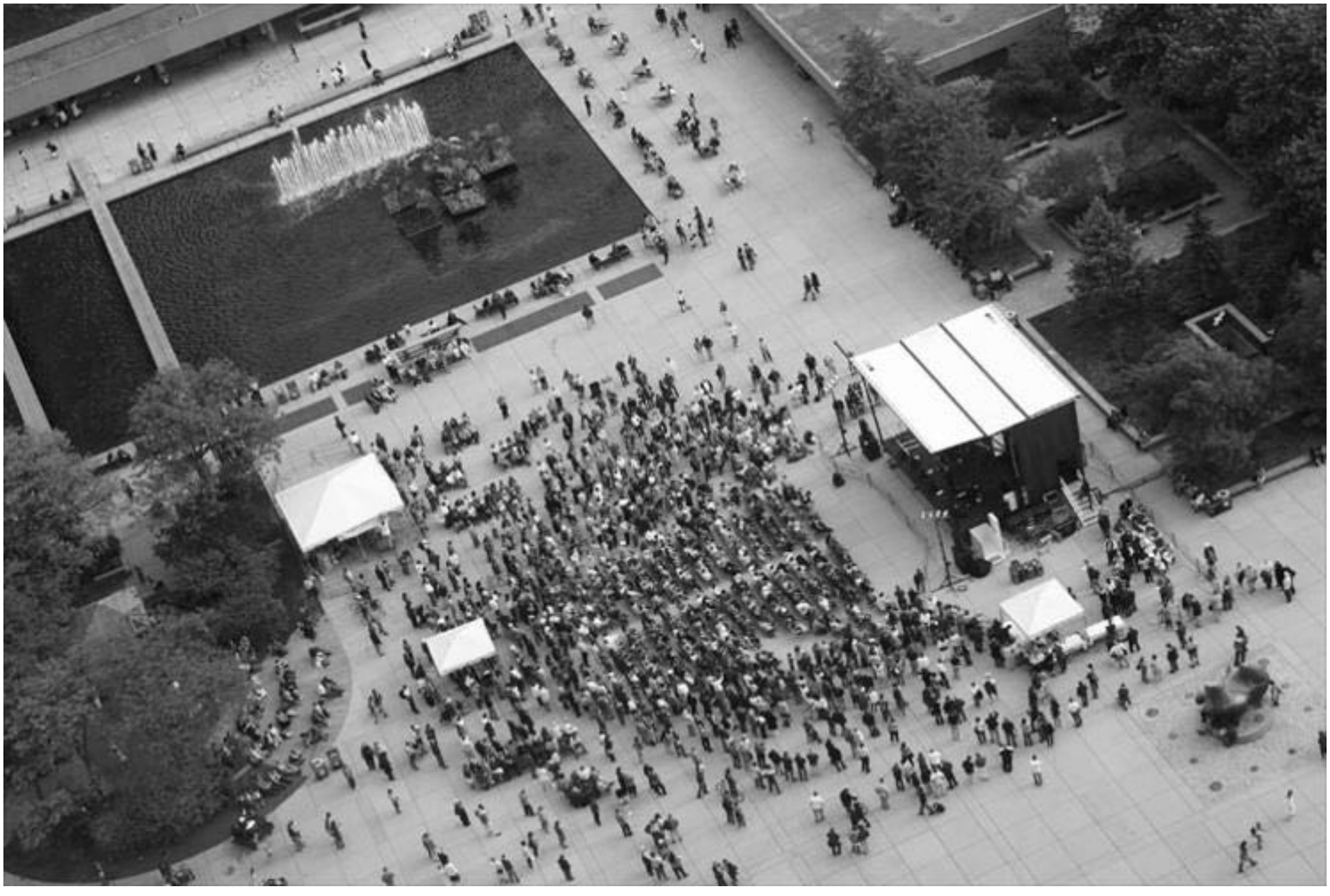
- 10 datasets (from UCI, DELVE and STATLOG repositories)
- Non binary problems partitioned into two-class problems.
- 100 partitions into test and training set (about 60%:40%).
- On each data sets we trained and tested all classifiers. Results are average test errors over 100 runs and standard deviations.
- Parameters estimated by 5-fold cross validation on first 5 realizations of dataset.
- For SVM we used Gaussian kernel
- For Boosting we used RBF networks as base learner

Real data

Experimental Results

	KNN	C4.5	RBF	AB	AB_R	SVM
Banana	$15.0_{\pm 1.0}$	$16.1_{\pm 2.8}$	$10.8_{\pm 0.6}$	$12.3_{\pm 0.7}$	$10.9_{\pm 0.4}$	$11.5_{\pm 0.7}$
B.Cancer	$28.4_{\pm 4.4}$	$24.6_{\pm 4.5}$	$27.6_{\pm 4.7}$	$30.4_{\pm 4.7}$	$26.5_{\pm 4.5}$	$26.0_{\pm 4.7}$
Diabetes	$28.9_{\pm 2.4}$	$26.0_{\pm 2.4}$	$24.3_{\pm 1.9}$	$26.5_{\pm 2.3}$	$23.8_{\pm 1.8}$	$23.5_{\pm 1.7}$
German	$28.9_{\pm 1.9}$	$28.1_{\pm 2.4}$	$24.7_{\pm 2.4}$	$27.5_{\pm 2.5}$	$24.3_{\pm 2.1}$	$23.6_{\pm 2.1}$
Heart	$15.8_{\pm 3.3}$	$20.4_{\pm 4.6}$	$17.6_{\pm 3.3}$	$20.3_{\pm 3.4}$	$16.5_{\pm 3.5}$	$16.0_{\pm 3.3}$
Ringnorm	$35.9_{\pm 1.3}$	$15.3_{\pm 1.5}$	$1.7_{\pm 0.2}$	$1.9_{\pm 0.3}$	$1.6_{\pm 0.1}$	$1.7_{\pm 0.1}$
F.Solar	$37.8_{\pm 2.8}$	$33.2_{\pm 1.9}$	$34.4_{\pm 2.0}$	$35.7_{\pm 1.8}$	$34.2_{\pm 2.2}$	$32.4_{\pm 1.8}$
Thyroid	$5.8_{\pm 2.8}$	$8.7_{\pm 3.3}$	$4.5_{\pm 2.1}$	$4.4_{\pm 2.2}$	$4.6_{\pm 2.2}$	$4.8_{\pm 2.2}$
Titanic	$25.5_{\pm 3.8}$	$22.9_{\pm 1.5}$	$23.3_{\pm 1.3}$	$22.6_{\pm 1.2}$	$22.6_{\pm 1.2}$	$22.4_{\pm 1.0}$
Waveform	$11.4_{\pm 0.8}$	$17.8_{\pm 1.0}$	$10.7_{\pm 1.1}$	$10.8_{\pm 0.6}$	$9.8_{\pm 0.8}$	$9.9_{\pm 0.4}$
Mean%	$2400_{\pm 6800}$	$1200_{\pm 2700}$	$5.8_{\pm 3.7}$	$13.4_{\pm 9.2}$	$2.7_{\pm 2.5}$	$2.9_{\pm 3.5}$

How many people?



Summary

- Ensemble learners combine simple learners to improve prediction.
- Easy to use.
- Typically perform well on real data.
- Based on intuitive concepts.
- But very strong links to theory and other methods (e.g. VC/SVM).

- Not much research anymore.
- But used in practice.

Margin

Theorem 2 *Suppose the base learning algorithm generates hypothesis with weighted training errors* $\epsilon_1, \ldots, \epsilon_T$. *Then we have for any* θ

$$P_{\mathbf{z}}(y f_{Ens}(\mathbf{x}) \leq \theta) \leq 2^T \prod_{t=1}^{T} \sqrt{{\epsilon_t}^{1-\theta}(1-\epsilon_t)^{1+\theta}}$$

Corollary 3 *If the base learning algorithm always achives* $\epsilon_t \leq \frac{1}{2} - \frac{1}{2}\gamma$ *then AdaBoost will generate a combined hyperplane with margin at least* $\frac{1}{2}\gamma$.

Margin bound

Theorem 4 *Let D be a distribution over $X \times \{\pm 1\}$ and let $\mathbf{Z}$ be a sample of N examples chosen independently at random according to D. Suppose the base-hypothesis space $\mathcal{H}$ has VC-dimension d, and let $\delta > 0$. Then with probability at least $1 - \delta$, the expected risk is bounded for $\theta > 0$ by*

$$R[f] \leq R^{\theta}_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{d \log^2\left(\frac{N}{d}\right)}{\theta^2 N} + \frac{\log(1/\delta)}{N}}\right)$$

Compare to SVMs:

$$R[f] \leq R_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{\log\left(N\theta^2\right)}{\theta^2 N} + \frac{\log(1/\eta)}{N}}\right).$$

- Bounds are independent of dimensionality of feature space