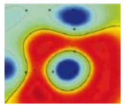
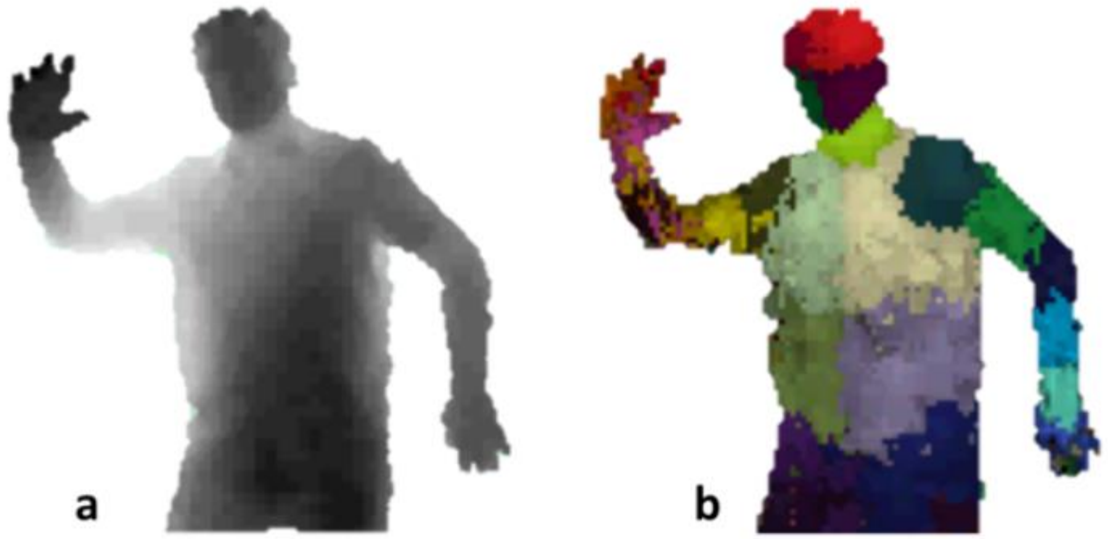
Decision Trees and Random Forrests

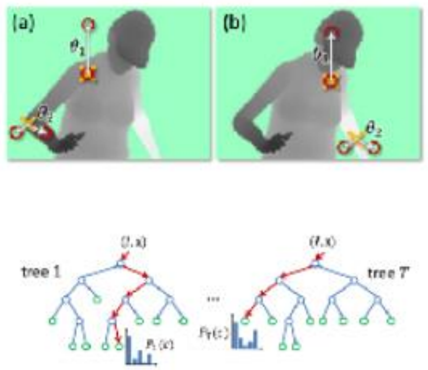
Klaus-Robert Müller



Tree-based Methods - applications

Microsoft Kinect Pose Estimation
(Classifications Forests in Kinect for XBox 360)





J. Shotton, A. Fitzgibbon, M. Cook, T. Sharp, M. Finocchio, R. Moore, A. Kipman, A. Blake. Real-Time Human Pose Recognition in Parts from a Single Depth Image (2011)

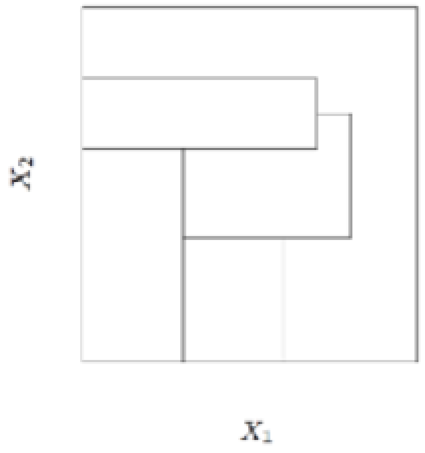
Tree-based Methods - applications

Other "real life" applications:

- Recommender systems (Facebook, Amazon, Netflix)
- Business applications (customer segmentation, target marketing)
- Medical (disease diagnosis)
- Banking (credit card issue, fraud detection)

Tree-based Methods - background

Given: Features: $X_1, X_2, \ldots, X_p$
Target: Y



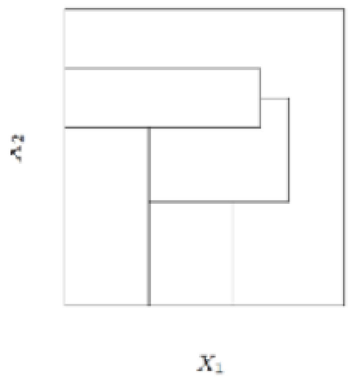
General Partition
(can not be obtained)

Key idea:

(1) Partition feature space into a set of rectangles.
(2) Fit a simple model (e.g. a constant) in each one.

For each partition: model Y with a different constant.

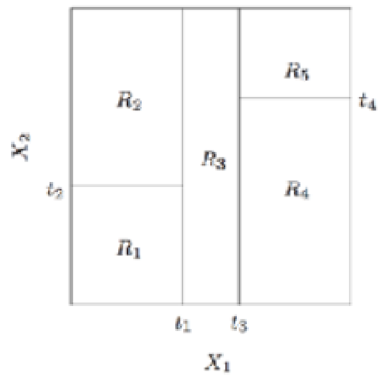
Tree-based Methods - background



General Partition
(can not be obtained)

Although each partitioning line has a simple description, e.g. X_1=c, some regions are complicated to describe.

Simplification: recursive binary partitions



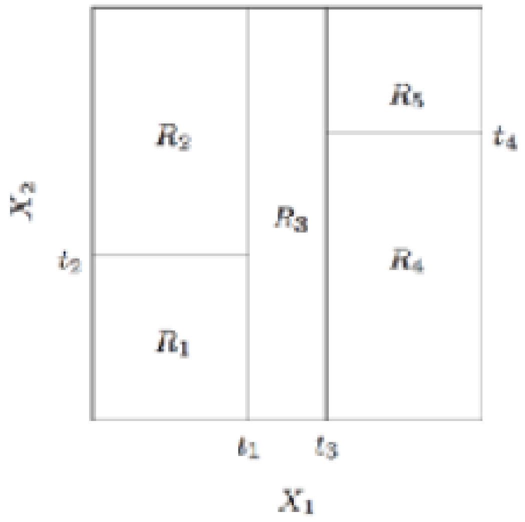
Recursive Binary Splitting

Algorithm (divide & conquer):

repeat
(1) Split space into two regions.
(2) Model response by mean of Y in each region.

The Elements of Statistical Learning, T. Hastie, R. Tibshirani, and J. Friedman (2001)

Decision Trees – conceptual construction



Recursive Binary Splitting

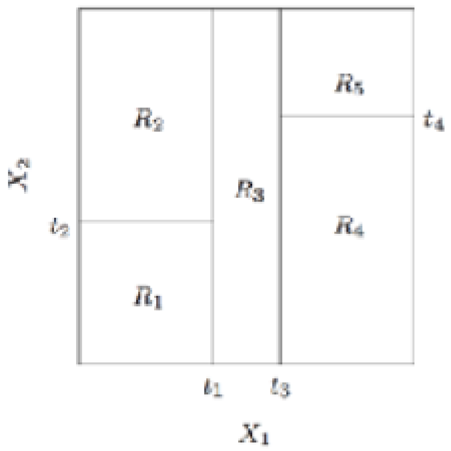
Example:

- Split at $X_1 = t_1$
- Split the region $X_1 <= t_1$ at t_2
- etc.

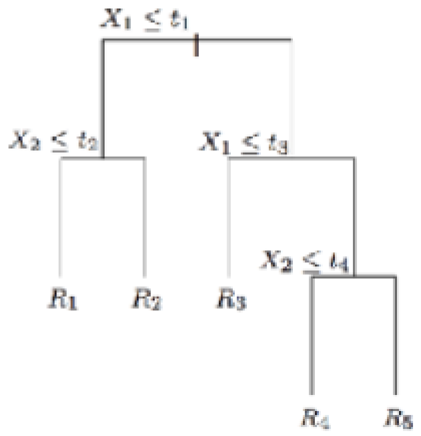
Result: Partitioning into R_1-R_5

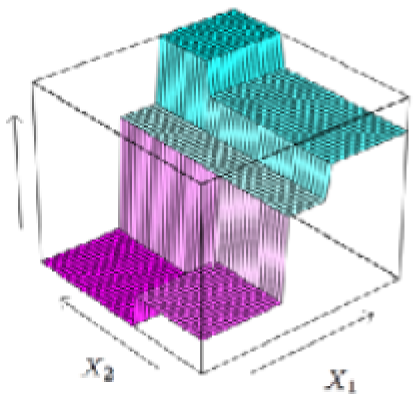
Model: $$\hat{f}(X) = \sum_{m=1}^{5} c_m I\{(X_1, X_2) \in R_m\}$$

Decision Trees – conceptual construction



Recursive
Binary Splitting





Decision Tree

Regression Surface

$$\hat{f}(X) = \sum_{m=1}^{5} c_m I\{(X_1, X_2) \in R_m\}$$

Decision Trees – algorithm

Given: *N* observations, *P* features

(x_i, y_i) for $i = 1, 2, \ldots, N$, with $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$.

Wanted: splitting variables *j*, split points *s*

(to partition space into M regions)

Minimization criterion: e.g. $\hat{c}_m = \text{ave}(y_i | x_i \in R_m)$ (sum of squares)

Finding best binary partition is computationally infeasible (NP hard): **use greedy approach**

Decision Trees – algorithm - splitting

Given: *N* observations, *P* features

$$(x_i, y_i) \text{ for } i = 1, 2, \ldots, N, \text{ with } x_i = (x_{i1}, x_{i2}, \ldots, x_{ip}).$$

Consider a splitting variable *j* and split point *s* and define a pair of half planes:

$$R_1(j,s) = \{X|X_j \le s\} \text{ and } R_2(j,s) = \{X|X_j > s\}$$

We seek *j* and *s* to solve:

$$\min_{j,\, s}\left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2\right]$$

Splitting:

Inner minimization solved by: $\hat{c}_1 = \text{ave}(y_i|x_i \in R_1(j,s))$ and $\hat{c}_2 = \text{ave}(y_i|x_i \in R_2(j,s))$

I.e. scan through all *P* features and determine optimal (j,*s*)

Decision Trees – algorithm – splitting (metrics)

Information gain

Based on the concept of entropy from information theory.

$$H(T) = I_E(p_1, p_2, \ldots, p_J) = -\sum_{i=1}^{J} p_i \log_2 p_i$$

were $p_1, p_2, \ldots$ represent the probability of each class present in the child node that results form splitting the tree.

$$\overbrace{IG(T,a)}^{\text{Information Gain}} = \overbrace{H(T)}^{\text{Entropy(parent)}} - \overbrace{H(T|a)}^{\text{Weighted Sum of Entropy(Children)}}$$

Choose the split that results in the purest daughter nodes.

Decision Trees – algorithm – splitting (metrics)

Gini impurtiy

Measure of how often a randomly chosen element from the set would be incorrectly labeled if it was randomly labeled according to the distribution of labels in the subset

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

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

Decision Trees – algorithm – splitting (metrics)

Variance Reduction (often used for regression)

Variance reduction of a node is defined as the total reduction of the variance of the target variable due to the split at this node.

$$I_V(N) = \frac{1}{|S|^2}\sum_{i\in S}\sum_{j\in S}\frac{1}{2}(x_i - x_j)^2 - \left(\frac{1}{|S_t|^2}\sum_{i\in S_t}\sum_{j\in S_t}\frac{1}{2}(x_i - x_j)^2 + \frac{1}{|S_f|^2}\sum_{i\in S_f}\sum_{j\in S_f}\frac{1}{2}(x_i - x_j)^2\right)$$

were S, S_t, and S_f are the set of pre-split sample indices for which the split test is true and false, respectively.

Decision Trees – algorithm – pruning

How large to grow the tree?

- too large: overfitting
- too small: not all important structure is captured

Solution: grow large tree, then prune using *cost-complexity criterion*

(collapse any number of internal (non-leaf) nodes)

$$N_m = \#\{x_i \in R_m\},$$ (training data in region)

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i,$$ (prediction in region)

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2,$$ (squared loss)

$$|T|$$ (number of terminal leaves)

$$\alpha \geq 0$$ (regularization parameter)

Find subtree that minimizes:

$$C_\alpha(T) = \sum_{m=1}^{|T|} \underbrace{N_m Q_m(T)}_{\text{cost}} + \underbrace{\alpha |T|}_{\text{complexity}}$$

Decision Trees – algorithm – pruning

Find subtree that minimizes:

$$C_\alpha(T) = \underbrace{\sum_{m=1}^{|T|} N_m Q_m(T)}_{\text{cost}} + \underbrace{\alpha|T|}_{\text{complexity}}$$

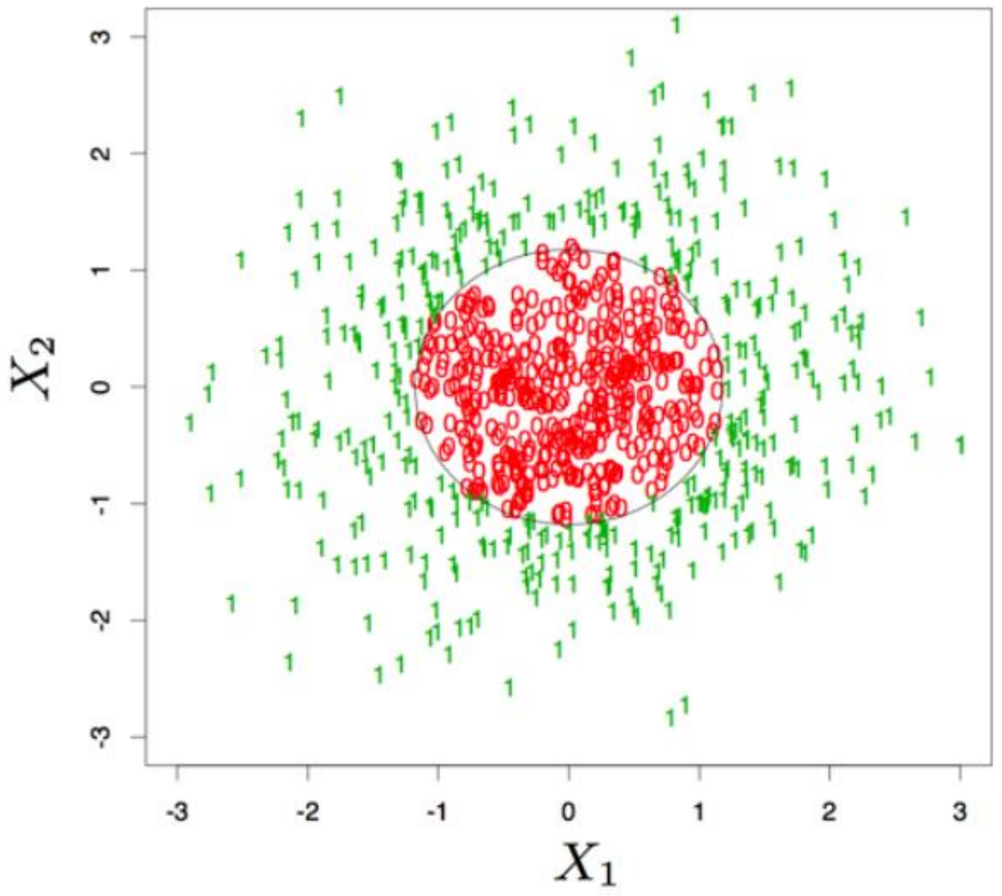
Weakest Link Pruning:

1. Starting with the full tree, successively collapse the internal node that produces the smallest per node increase in $\sum_m N_m Q_m(T)$

   Result: Sequence of trees $T_0, T_1, T_2, \ldots, T_m$ (were T_m is a single-leaf tree)

2. Choose optimal α (the optimal tree T_i) via cross-validation.

Toy Classification Problem - setup



Given: *N* training pairs (X_i, Y_i)

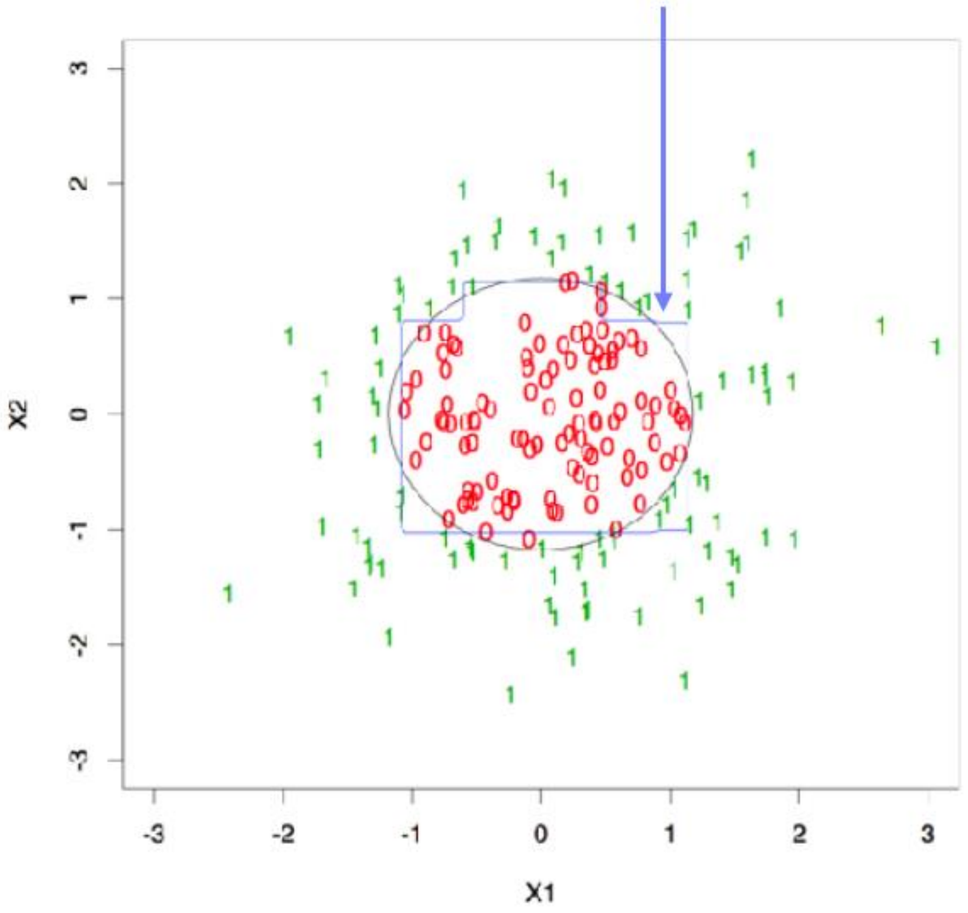
(black line: optimal decision boundary)

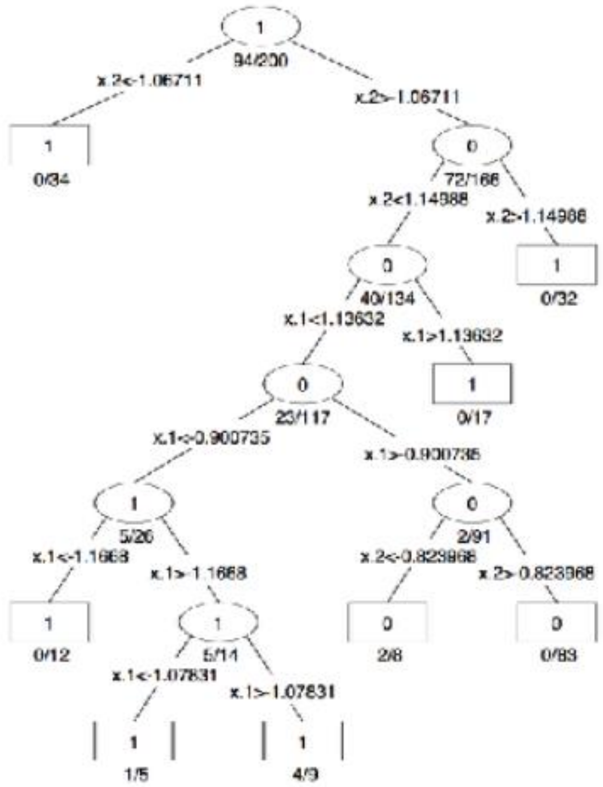
Goal: Produce a classifier

$$\hat{C}(X) \in \{-1, 1\}$$

Toy Classification Problem - result

$\hat{C}(X)$ is rather noisy!





Classification Tree

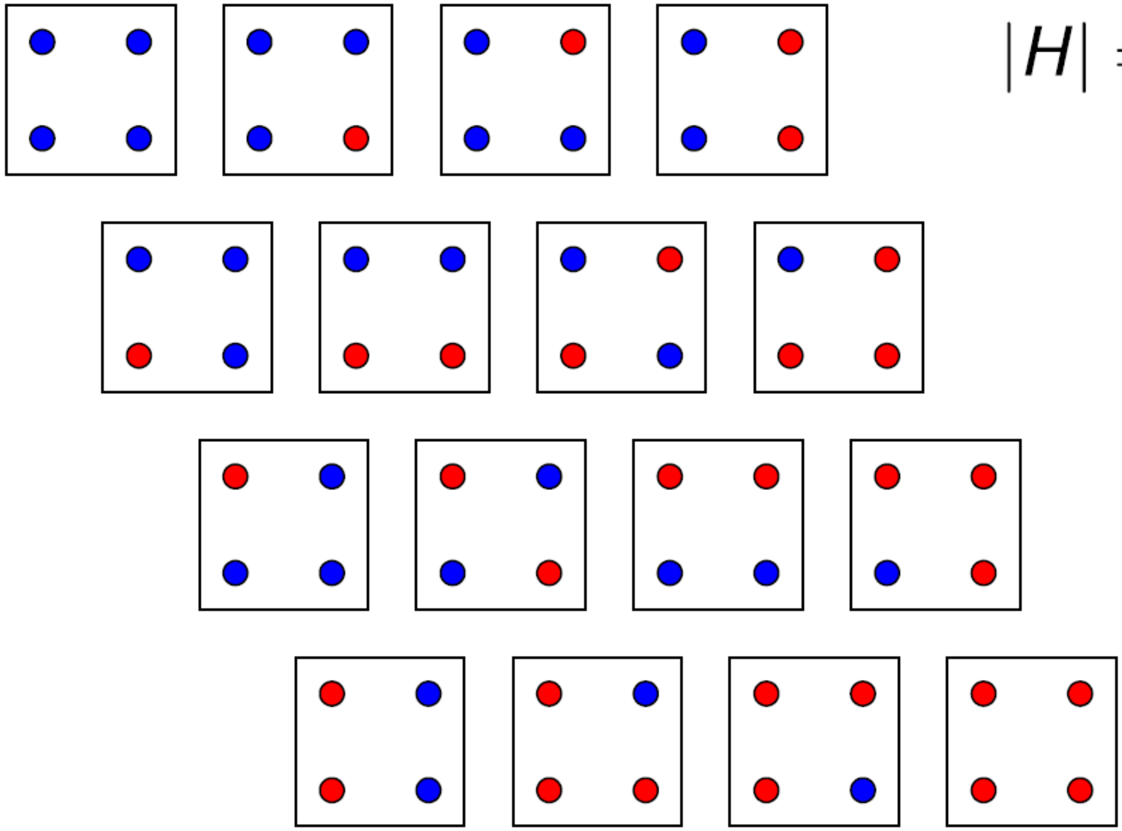
Decision Trees- advantages

- Interpretability
- Generalizes to higher dimensions
- Can handle mixed predictors: quantitative & qualitative
- Easily ignores redundant variables
- Handles missing data elegantly

BUT: decision trees are prone to overfitting (high variance)

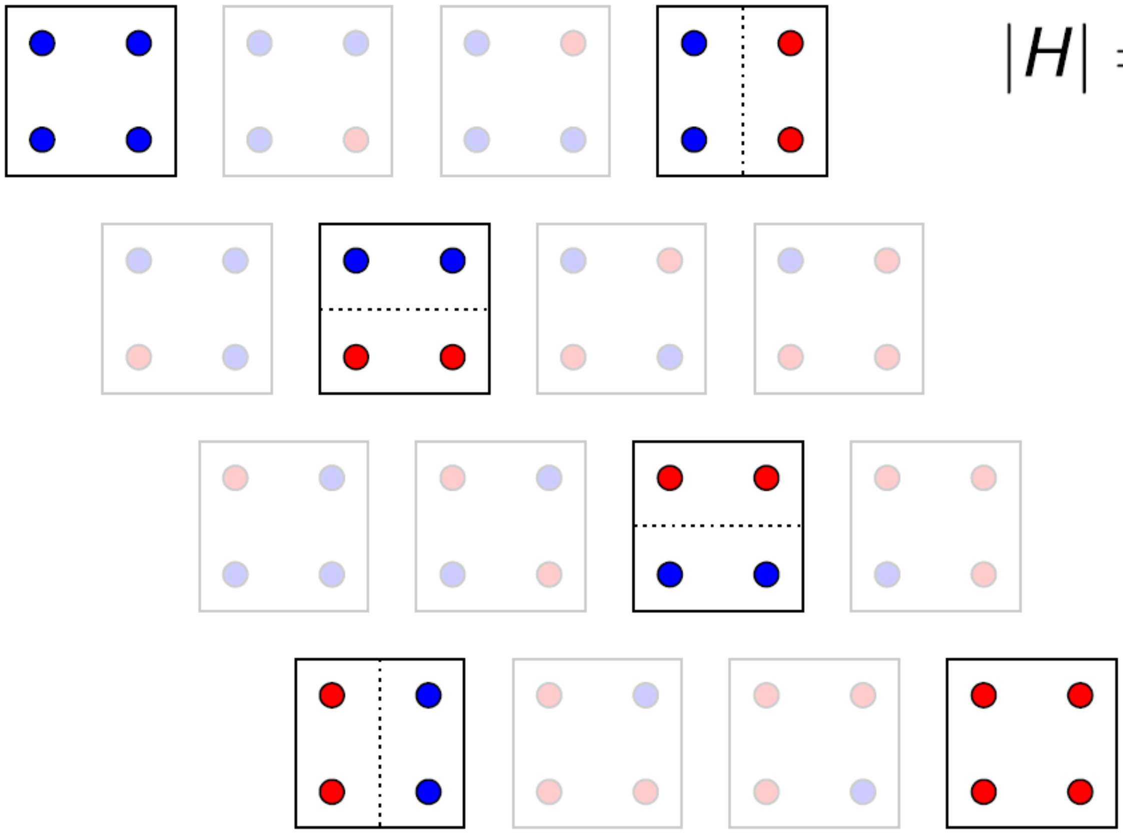
learning theory for decision trees

Hypothesis Space – general classifiers



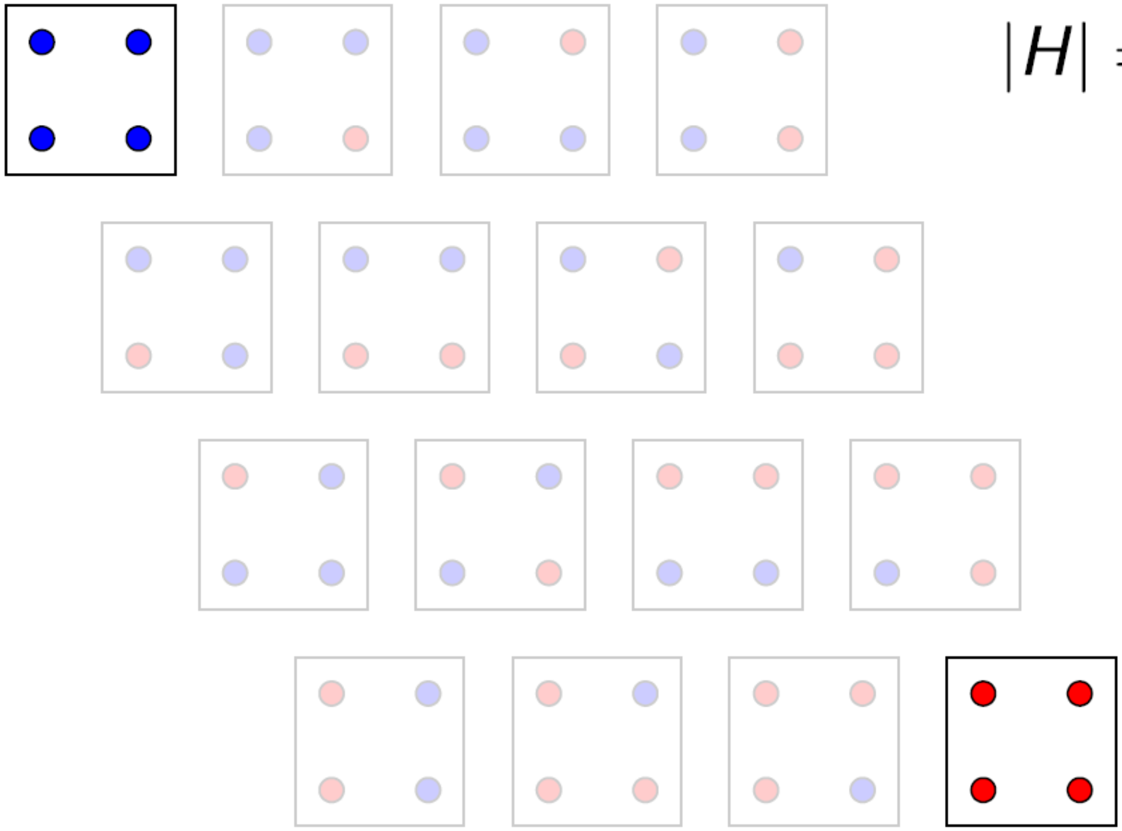
$|H| = 16$

Hypothesis Space – decision trees (level 1)



$$|H| = 6$$

Hypothesis Space – constant classifiers



$$|H| = 2$$

Bounding Generalization Error

[Haussler'88]: When the hypothesis space H is finite, then, the generalization error of a consistent (i.e. correctly classifying) hypothesis h can be bounded as:

$$P(\mathrm{error}_{\mathcal{X}}(h) > \varepsilon) \leq |H| e^{-m\varepsilon}$$

... where $|H|$ is the size of the hypothesis space, and m is the number of iid samples in the training set.

Observation: generalization error grows with the number of hypotheses and decreases with the number of data points.

Bounding Generalization Error

If we take the bound from the previous slide and consider the probability to be constant

$$\underbrace{P(\mathrm{error}_{\mathcal{X}}(h) > \varepsilon)}_{\delta} \leq |H| e^{-m\varepsilon}$$

then, we can rewrite the bound in a more convenient way as

$$\mathrm{error}_{\mathcal{X}}(h) \leq \frac{\log |H| + \log \frac{1}{\delta}}{m}$$

i.e. generalization error grows with model complexity $|H|$ and decreases with the training set size m.

Bounding Generalization Error

Limitation of Haussler's bound:

- It applies only to set of hypotheses that perfectly classify the data. What if we use a simple model (e.g. shallow decision tree or linear classifier?)

Another bound (derived from the Chernoff inequality) for the generalization error is given by:

$$\text{error}_{\mathcal{X}}(h) \leq \underbrace{\text{error}_{\mathcal{D}}(h)}_{\substack{\text{training error} \\ \sim \textbf{bias}}} + \underbrace{\sqrt{\frac{\log|H| + \log\frac{1}{\delta}}{2m}}}_{\substack{\text{error due to} \\ \text{model complexity} \\ \sim \textbf{variance}}}$$

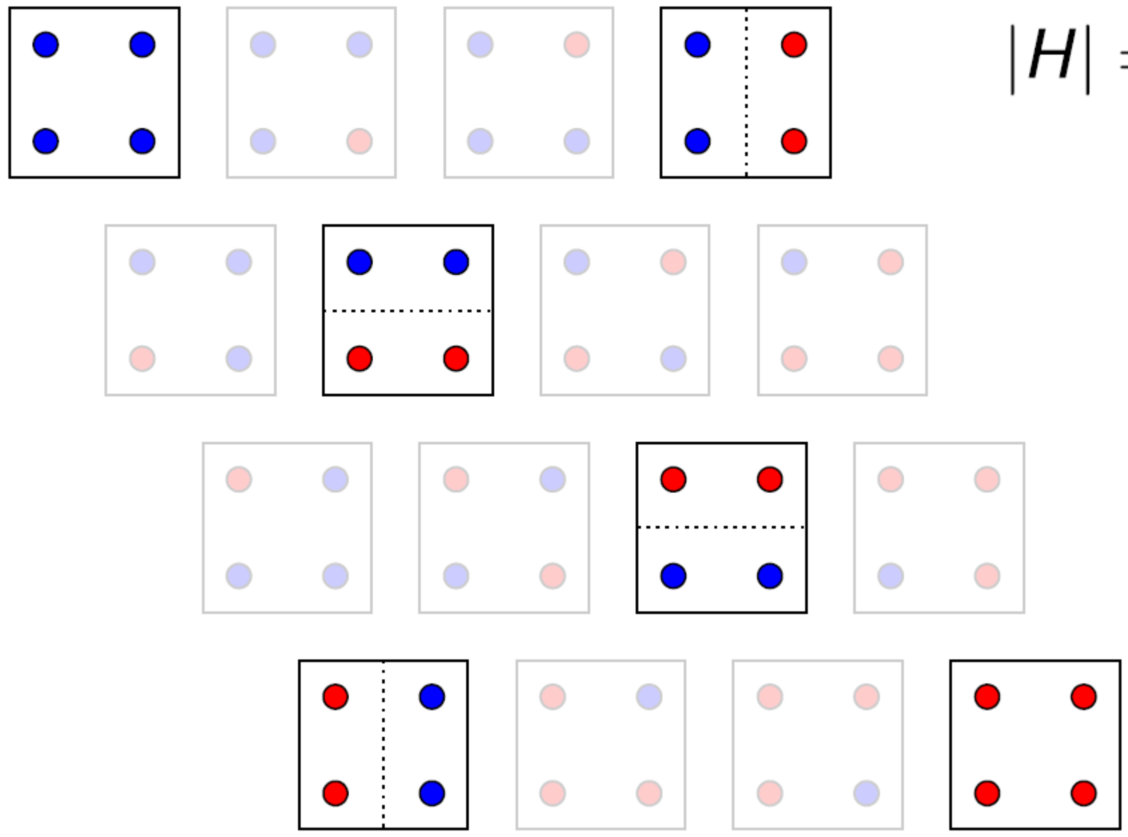
Application to Decision Trees

Question: Can we bound the error of decision trees?

How large is the hypothesis space of decision trees?

$$\text{error}_{\mathcal{X}}(h) \leq \underbrace{\text{error}_{\mathcal{D}}(h)}_{\sim \text{ bias}} + \underbrace{\sqrt{\frac{\log|H| + \log\frac{1}{\delta}}{2m}}}_{\sim \text{ variance}}$$

Hypothesis Space – decision trees (level 1)



$|H| = 6$

Complexity of Decision Trees

- **Example 1:** General decision tree with n binary features (i.e. expanded until it perfectly classifies data):

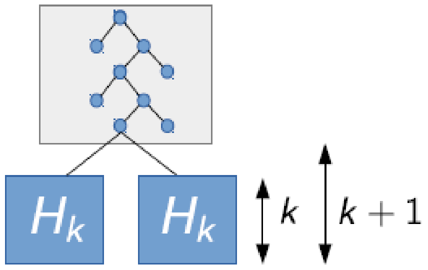
$|H| = 2^{2^n}$ i.e. all possible lookup tables over n binary features.

- **Example 2:** Decision tree of depth 0:

$|H| = 2$ H $= \{$always labeling "0", always labeling "1"$\}$

Complexity of Decision Trees

Solution for trees of depth k: Use induction



- Initial condition: $|H_0| = 2$
- Recursion: $|H_{k+1}| = n \times |H_k| \times |H_k|$

$$\underbrace{n}_{\text{choice of root attribute}} \quad \underbrace{|H_k|}_{\text{left tree}} \quad \underbrace{|H_k|}_{\text{right tree}}$$

- Result $\log_2 |H_k| = (2^k - 1)(1 + \log_2 n) + 1$

Wrap-up

How large is the hypothesis space of decision trees?

$$\mathrm{error}_{\mathcal{X}}(h) \leq \underbrace{\mathrm{error}_{\mathcal{D}}(h)}_{\sim \text{ bias}} + \underbrace{\sqrt{\frac{\log|H| + \log\frac{1}{\delta}}{2m}}}_{\sim \text{ variance}}$$

Decision tree:

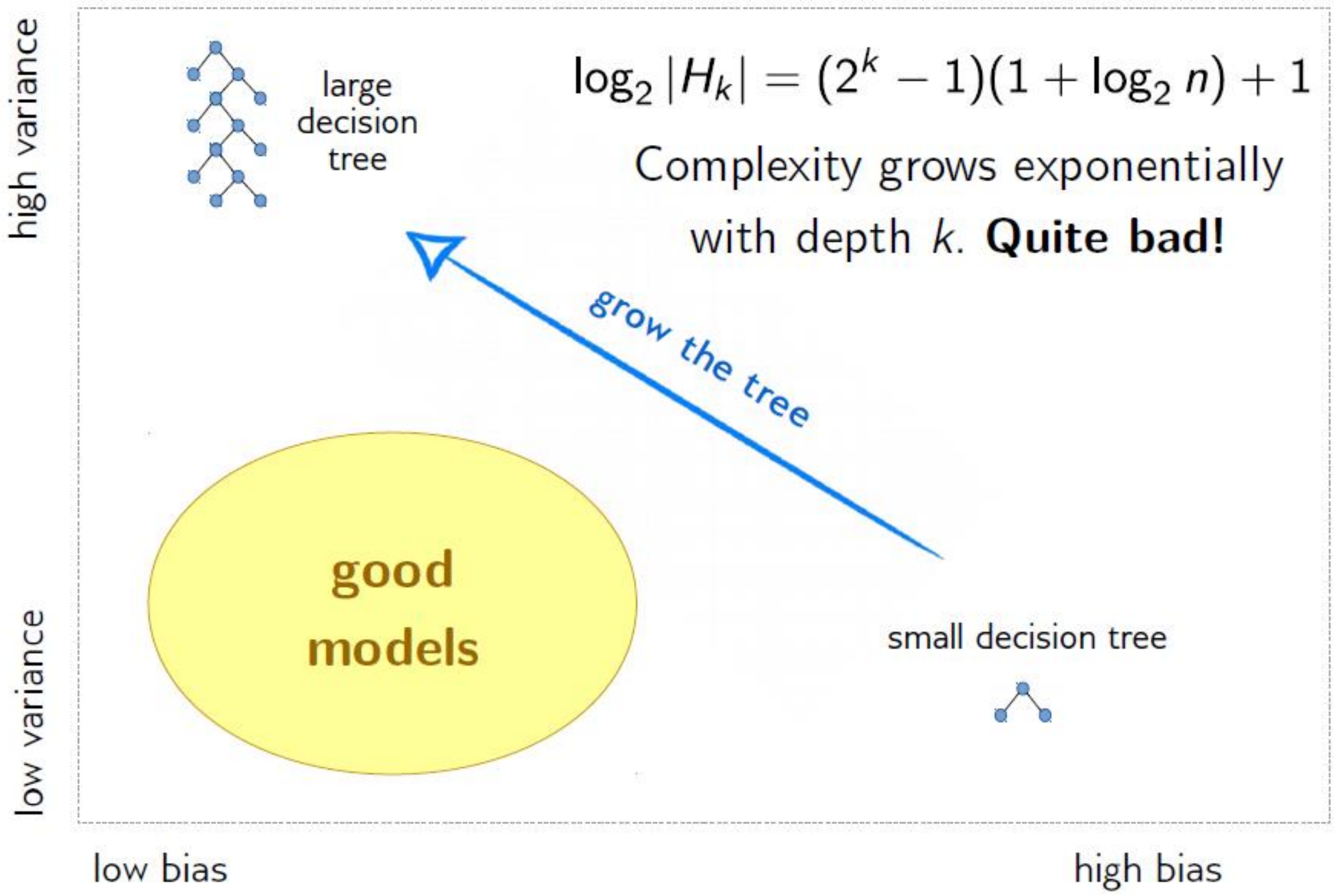
- Depth 0 (constant labeling) $\log_2|H_0| = 1$
- Depth k $\log_2|H_k| = (2^k - 1)(1 + \log_2 n) + 1$
- Unrestricted $\log_2|H| = 2^n$

high bias / low variance

$\downarrow \uparrow$

low bias / high variance

Decision Trees and Bias Variance


high variance
low variance
large decision tree
$\log_2 |H_k| = (2^k - 1)(1 + \log_2 n) + 1$
Complexity grows exponentially with depth k. **Quite bad!**
grow the tree
good models
small decision tree
low bias
high bias

$\rightarrow$ **We need better capacity control.**

Idea: combine decision trees with averaging, boosting.

DT- regularization via model averaging (ensembles)

Generalization error: $\mathrm{E}\left[\left(y-\hat{f}(x)\right)^2\right] = \mathrm{Bias}\left[\hat{f}(x)\right]^2 + \mathrm{Var}\left[\hat{f}(x)\right] + \sigma^2$

bias: low (if sufficiently deep)

+ **variance:** high (sensitive to choice of splits)

+ **residual error**

Consequence: decision trees often produce <u>noisy or weak</u> classifiers!

Idea: Combine the predictions of several randomized trees into single model.

Toy Classification Problem

Bagging (**B**ootstrap **agg**rega**t**ing)

Classifier $C(\mathcal{S}, x)$
training data S

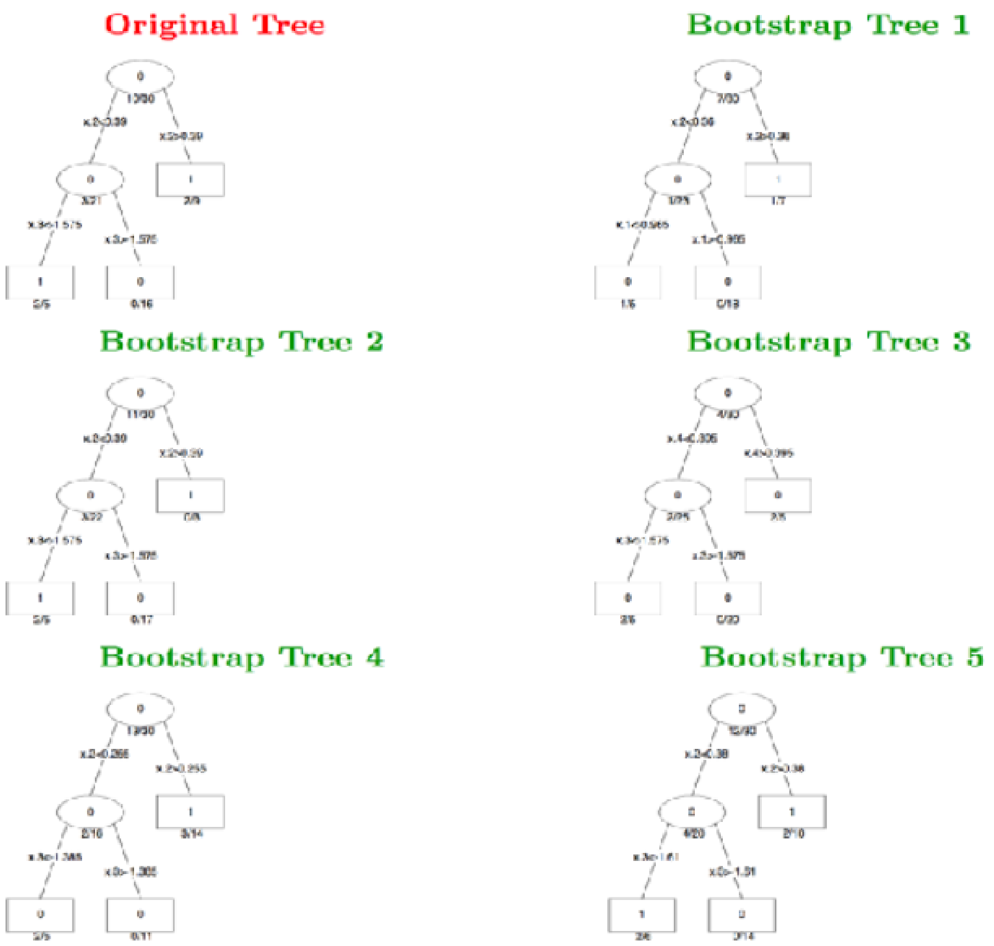
Train B models on different dataset:

Draw $\mathcal{S}^{*1}, \ldots \mathcal{S}^{*B}$
samples sets of length *N*
(bootstrap samples: duplicates allowed!)

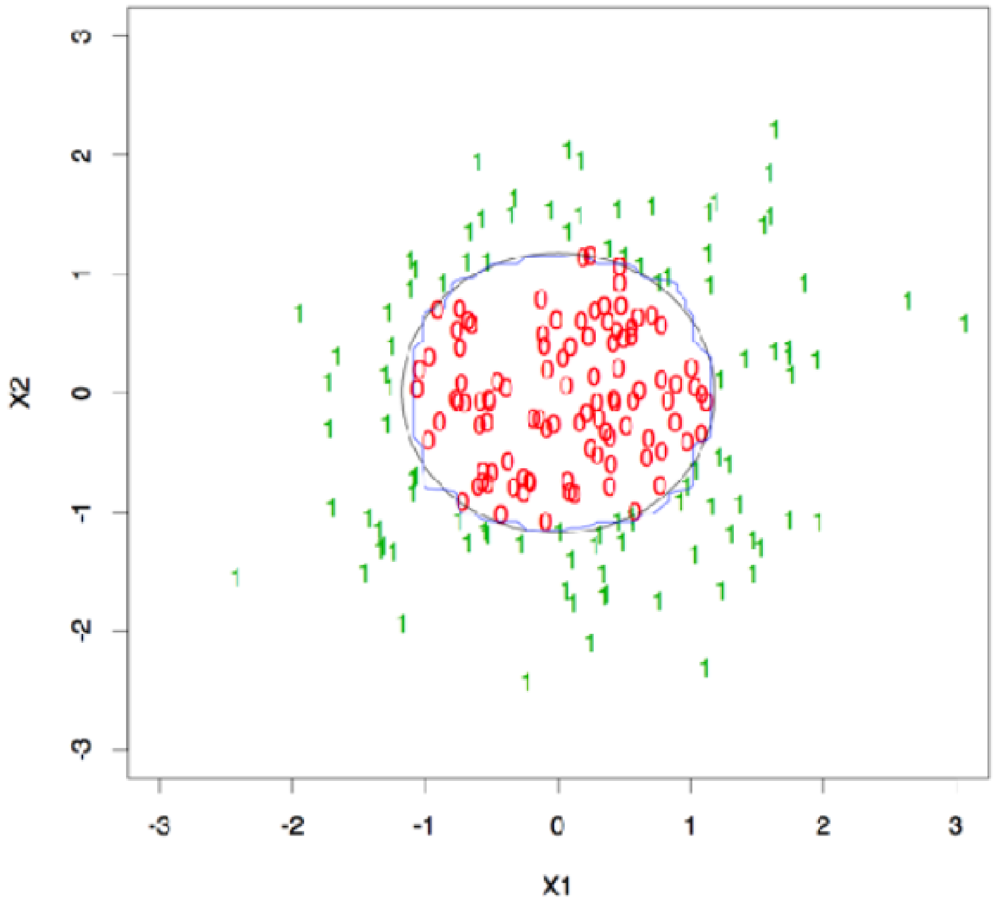
Prediction:

$$\hat{C}_{bag}(x) = \text{Majority Vote } \{C(\mathcal{S}^{*b}, x)\}_{b=1}^{B}$$

(in classification; regression: avergage)



Toy Classification Problem - bagging



Improved prediction via reduced variance

Bagging averages trees for smoother decision boundaries.

Bagging - limitations

- **Datasets highly overlapping:**
  Predictions of different trees become highly correlated.

- **Variance not reduced as much as desired!**

Random Forrests - overview

Random Subspace Method **(Tin Kam Ho, 1998):**
Randomly sample features $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ without replacement

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

Random Forest **(Breiman, 1999):**
Combination of Bagging + Random Subspace Method applied to decision trees

- Complexity control through “out-of-bag” control
  (estimate generalization error using untrained samples)
- Random feature selection either at tree or split level

Random Forrests - algorithm

For *b* = *1* to *B*:

(a) Draw a <u>bootstrap sample</u> (random sampling with replacement) of size *N* from the training data.

(b) Grow a tree T_b to the bootstrapped data until minimum node size reached:

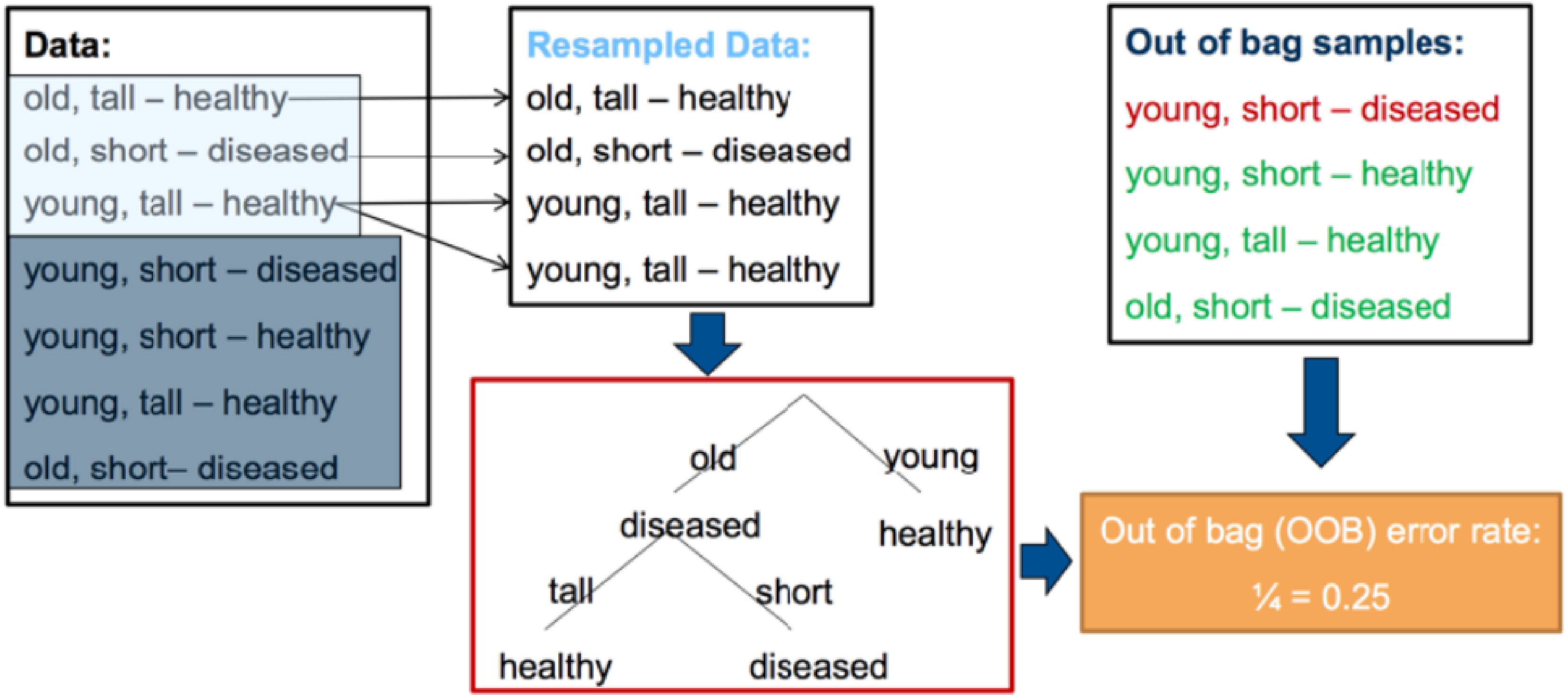
- i. Select *m* features at random.
- ii. Pick best variable/split-point among the *m*.
- iii. Split node into two daughter nodes.

Result: ensemble of *B* trees.

Prediction: $\hat{f}^B_{\text{rf}}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$ (regression)

$\hat{C}^B_{\text{rf}}(x) = \mathit{majority\ vote}\ \{\hat{C}_b(x)\}_1^B$ (classification)

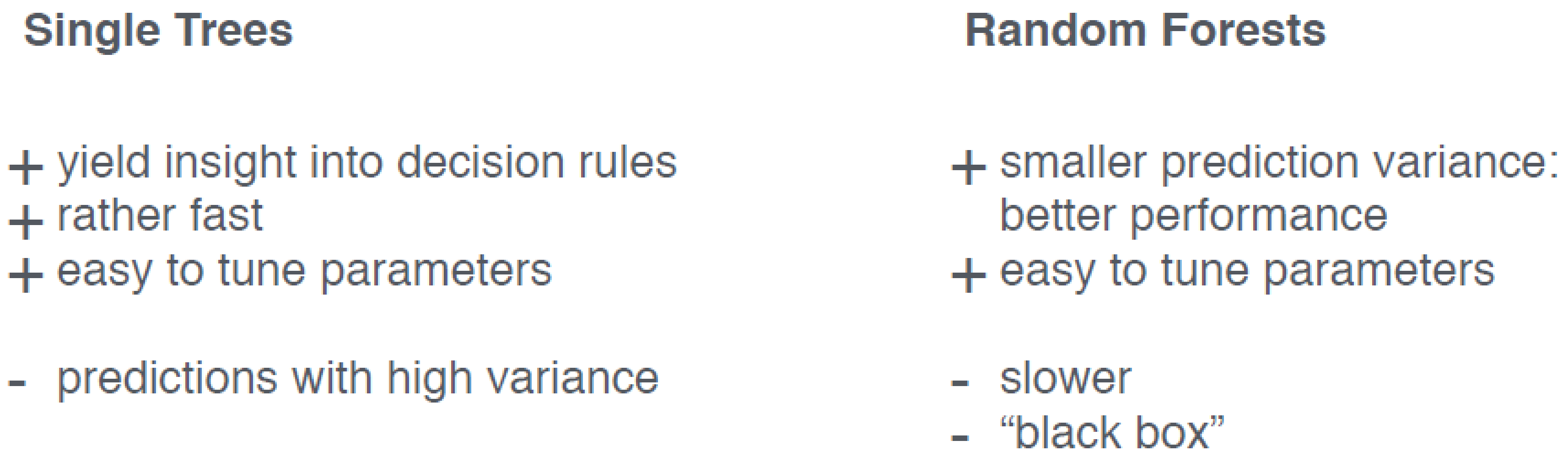
Random Forrests - algorithm



Random Forrests – differences to single tree

- Train each tree on bootstrap resample of data.
- For each split: consider only a subset of *m* randomly selected features. (typically $m = \sqrt{p}$ or $\log_2 p$ were p is the total number of features)
- No pruning.
- Fit *B* trees this way and aggregate predictions.

Random Forrests – differences to single tree



Single Trees

+ yield insight into decision rules
+ rather fast
+ easy to tune parameters

- predictions with high variance

Random Forests

+ smaller prediction variance: better performance
+ easy to tune parameters

- slower
- “black box”

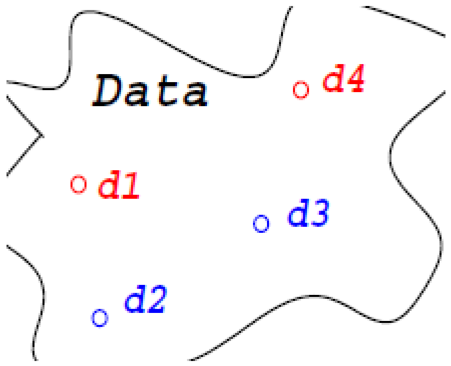
Boosting - conceptually

Idea: given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote.

On each iteration:

- Like in bagging, draw a sample of the observations from data (with replacement).
- Unlike in bagging, observations are not sampled randomly
  Higher weight observations are more likely chosen.
- Weight each training example by how incorrectly it was classified.
  Weight is higher for examples that are harder to classify.

The Adaboost Algorithm



Input: N examples $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

Initialize: $d_i^{(1)} = 1/N$ for all $i = 1 \ldots N$

Do for $t = 1, \ldots, T$,

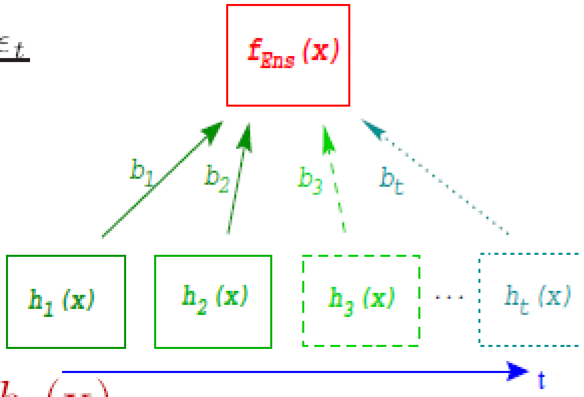
1. Train base learner according to example distribution $\mathbf{d}^{(t)}$ and obtain hypothesis $h_t : \mathbf{x} \mapsto \{\pm 1\}$.

2. compute weighted error $\epsilon_t = \sum_{i=1}^{N} d_i^{(t)} \mathrm{I}(y_i \neq h_t(\mathbf{x}_i))$

3. compute hypothesis weight $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$

4. update example distribution

$$d_i^{(t+1)} = d_i^{(t)} \exp\left(-\alpha_t y_i h_t(\mathbf{x}_i)\right) / Z_t$$



Output: final hypothesis $f_{\mathrm{Ens}}(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})$

Gradient Tree Boosting - conceptually

Idea: Iteratively improve a weak learner by correcting it: $F_{m+1}(x) = F_m(x) + h(x)$

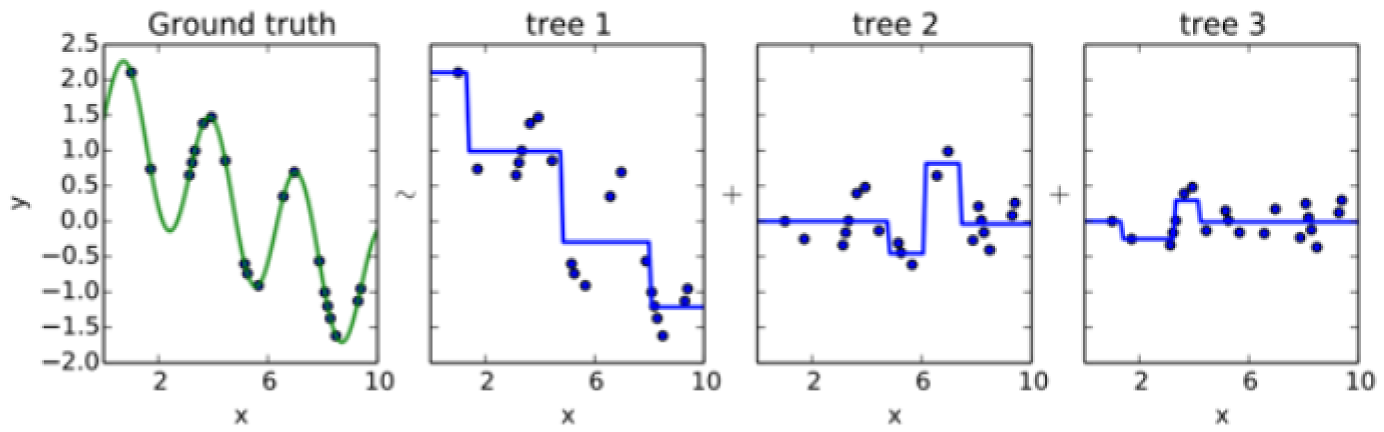
A perfect correction h(x) implies: $F_{m+1}(x) = F_m(x) + h(x) = y$

i.e. $h(x) = y - F_m(x)$

Hence we fit a new tree to the residual: $y - F_m(x) \longrightarrow \frac{1}{2}(y - F(x))^2$

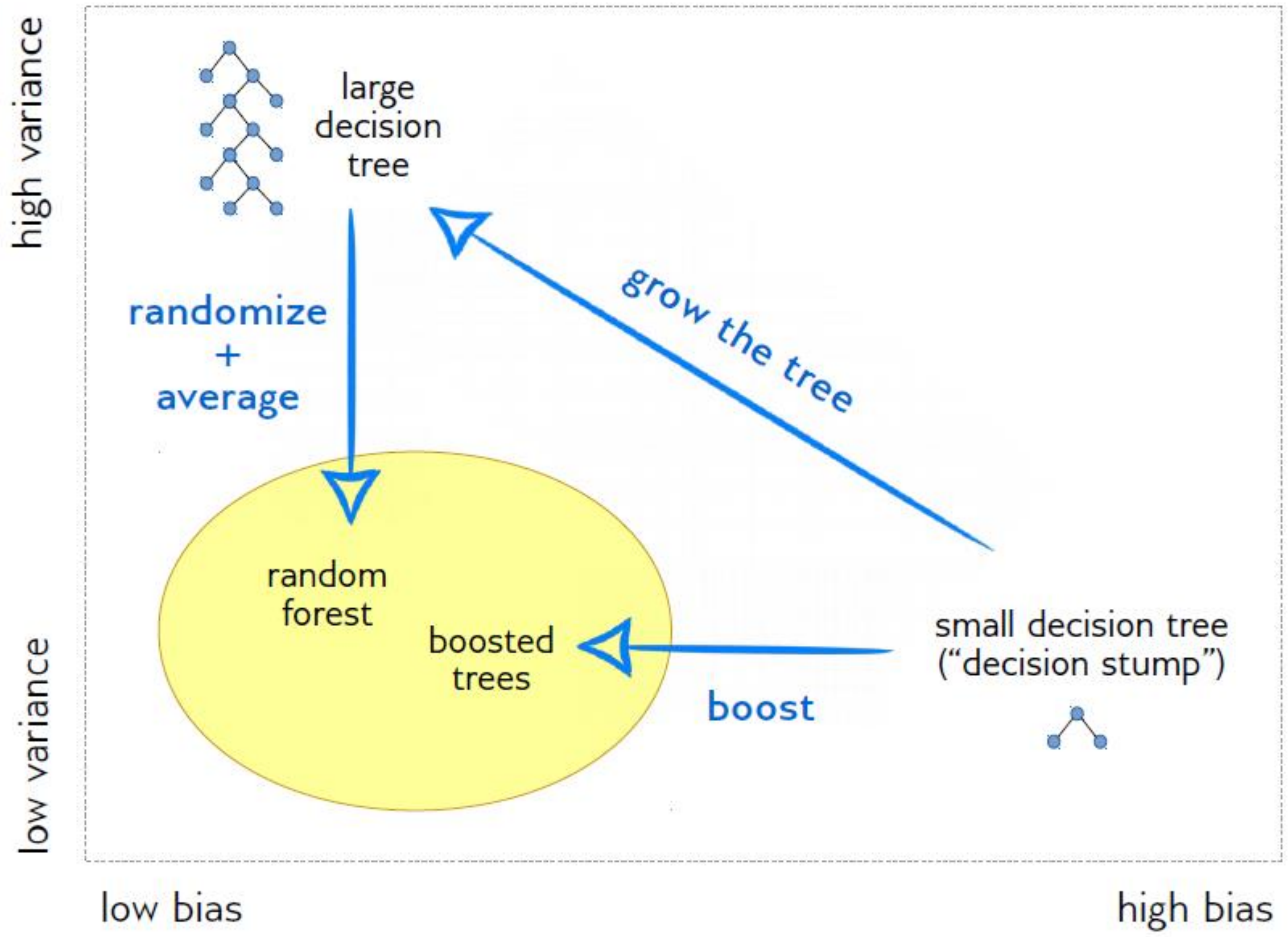
(negative gradient of quadratic loss function)

Residual fitting:



Gradient boosting is a <u>gradient descent</u> algorithm and can be trivially <u>generalized with other loss functions</u> and their gradients.

Decision Trees and Bias Variance


high variance
low variance
large decision tree
randomize + average
grow the tree
random forest
boosted trees
boost
small decision tree ("decision stump")
low bias
high bias