Statistical Learning– MATH 6333
Set 6 (Tree-Based Methods)

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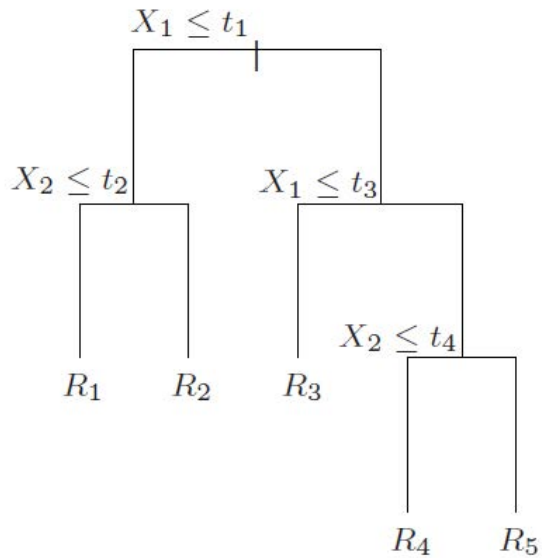
Tree-Based Methods

Classification and Regression Tree (CART)

- Another method for regression (Y is continuous) and classification (Y is categorical).
- It produces recursively a binary partition of the input space with constant predicted outputs c_m for R_m.
- The predicted regression surface

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



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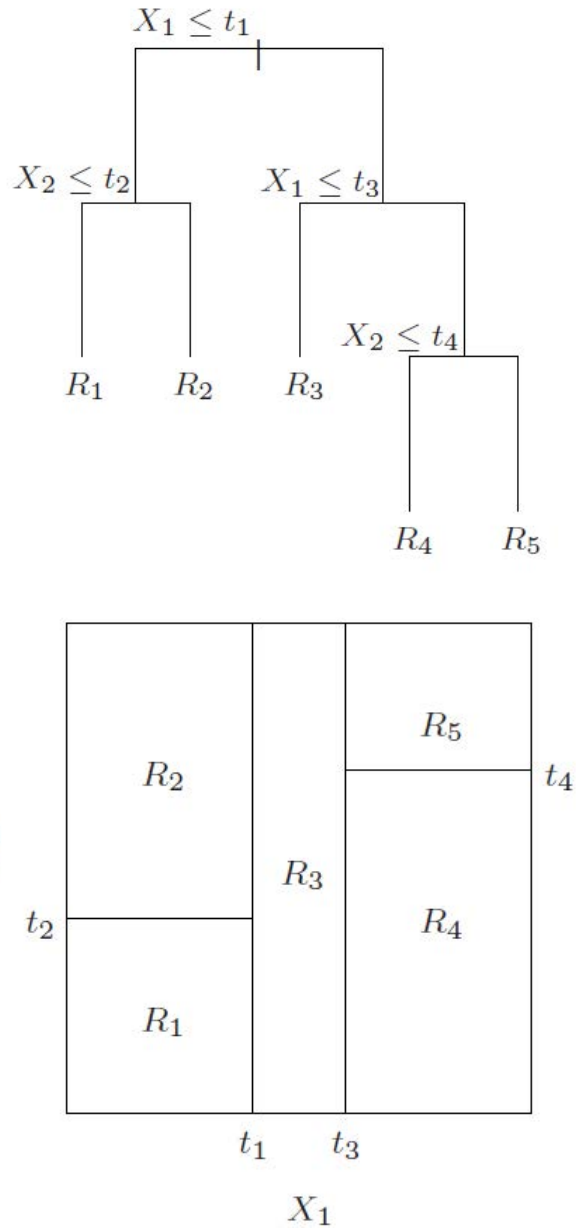

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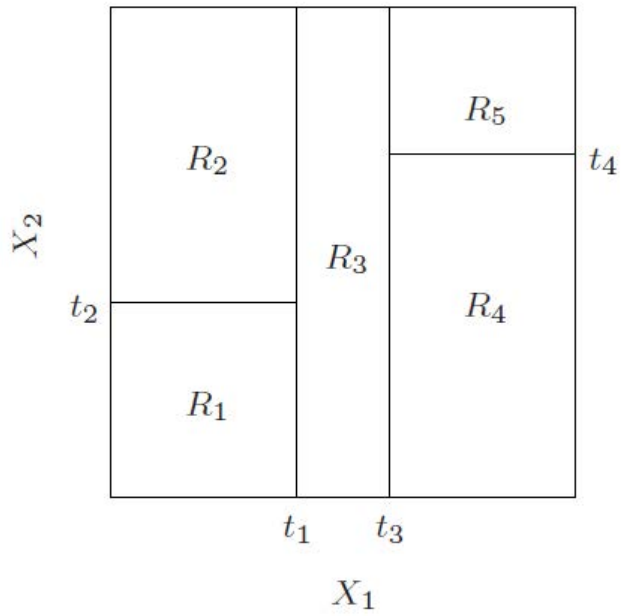

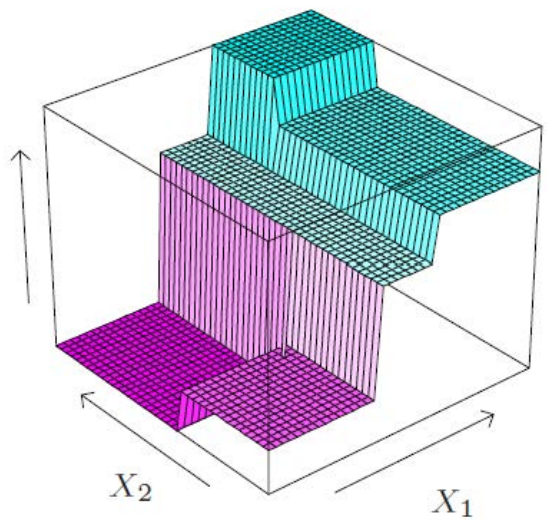

Regression Trees

Regression Trees

- If Y is continuous, then $\hat{c} = \{\hat{c}_m, m = 1, 2, \ldots, M\}$ could be found using the method of least squares by minimizing

$$RSS(c) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$

- It results in

$$\hat{c}_m = average(y_i | x_i \in R_m) = \frac{1}{N_m} \sum_{i: x_i \in R_m} y_i$$

  where $N_m = |\{i : x_i \in R_m\}|$

- But, finding the binary partition $\{R_m, m = 1, 2, \ldots, M\}$ is computationally infeasible.
- Unless, we use a greedy (short-sighted) algorithm to "grow a regression tree top-down."

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Regression Trees

Recursive binary splitting

- selecting variable X_j and cut-off point s that define the two regions

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

- Then find optimal j, s using that minimize RSS

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

- Internally, for the optimal j, s,

$$\hat{c}_1 = average(y_i | x_i \in R_1(j,s))$$

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The algorithm continues by

- dividing one of the resulting regions into further two divided regions via similar optimization problem and then
- further divide one of the resulting three regions and so on and so forth till there is no more than 5 observations in each region.
- But, when to stop growing the tree? (Large trees lead to overfitting, and small trees are less effective.)
- May be using a threshold for RSS below which the algorithm stops splitting. But early sub-optimal stopping is possible.
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Regression Trees

Tree Pruning

Stopping and pruning goes by

- growing a tree T_0 and stop splitting when a selected minimum node size is reached.
- Prune the tree using a cost-complexity pruning, *aka* weakest link pruning. (Pruning works backward by collapsing internal (non-terminal) nodes back to get a subtree $T \subset T_0$.) Let $|T|$ be the number of terminal nodes in T.
- Find tuning parameter $\alpha \geq 0$ (by CV) and the subtree $T_\alpha \subset T_0$ that minimize the cost complexity criterion

$$C_\alpha(T) = \sum_{m=1}^{|T|} + \alpha|T|$$

where $\hat{c}_m = \frac{1}{N_m} \sum_{i:x_i \in R_m} y_i$ and $N_m = |\{i : x_i \in R_m\}|$.

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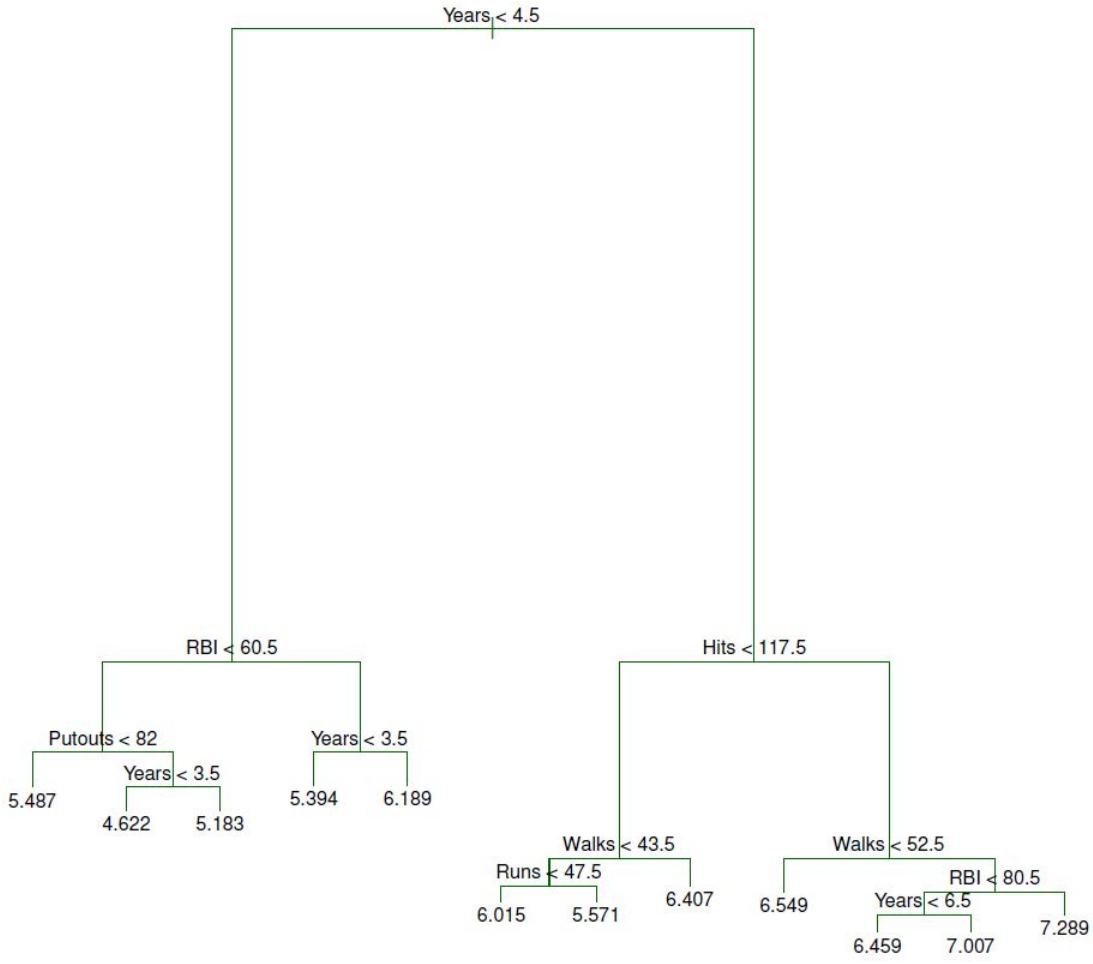
Regression Trees

Example (Hitters data)

To predict baseball player's Salary ($Y = \log(\text{Salary}/1,000)$) based on Years in a major league and previous year's number of Hits, etc., RT gives T_0



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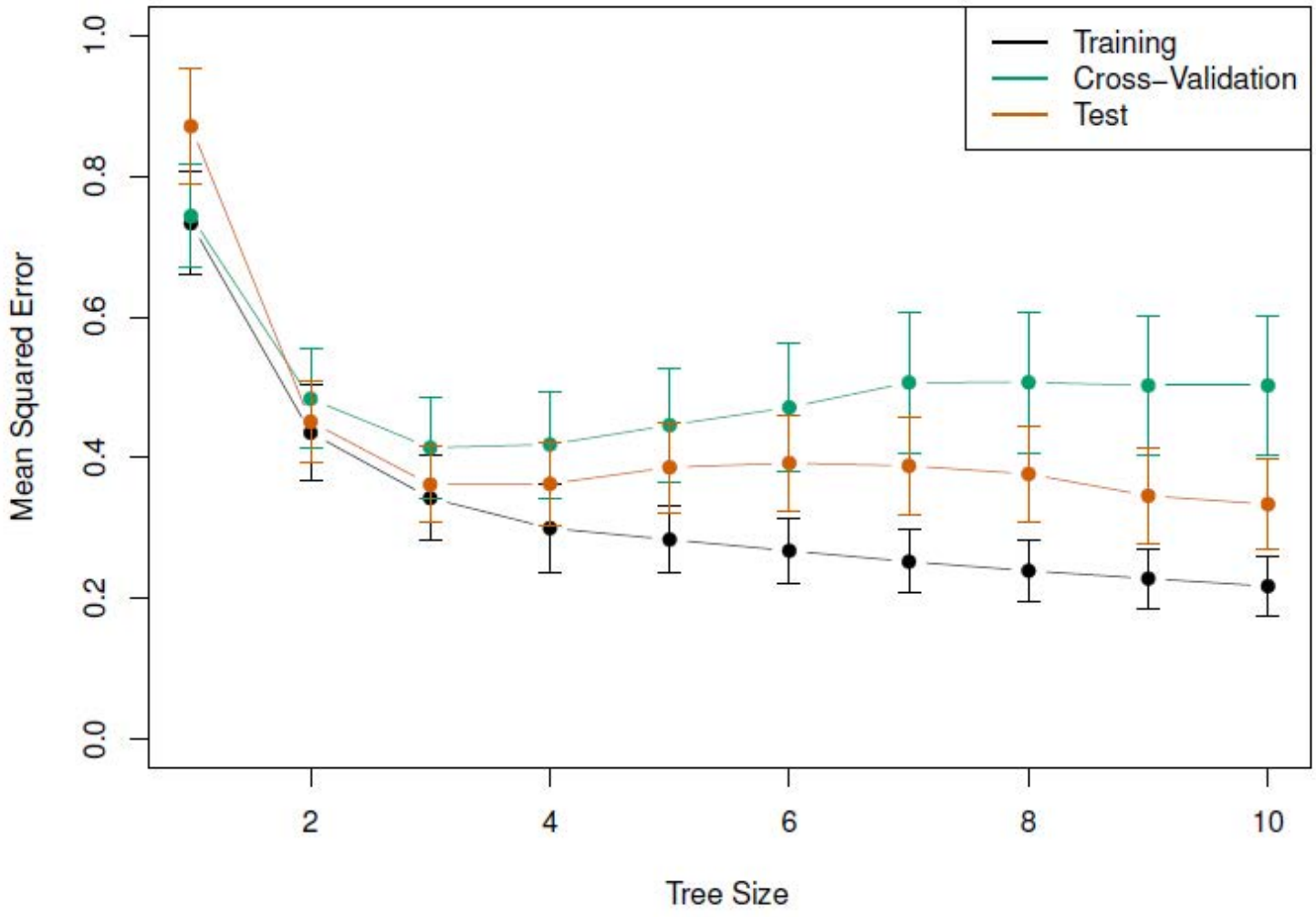
Example (Hitters data)

A cross-validation will find the optimal tree size $|T| = 3$ (number of terminal nodes.)



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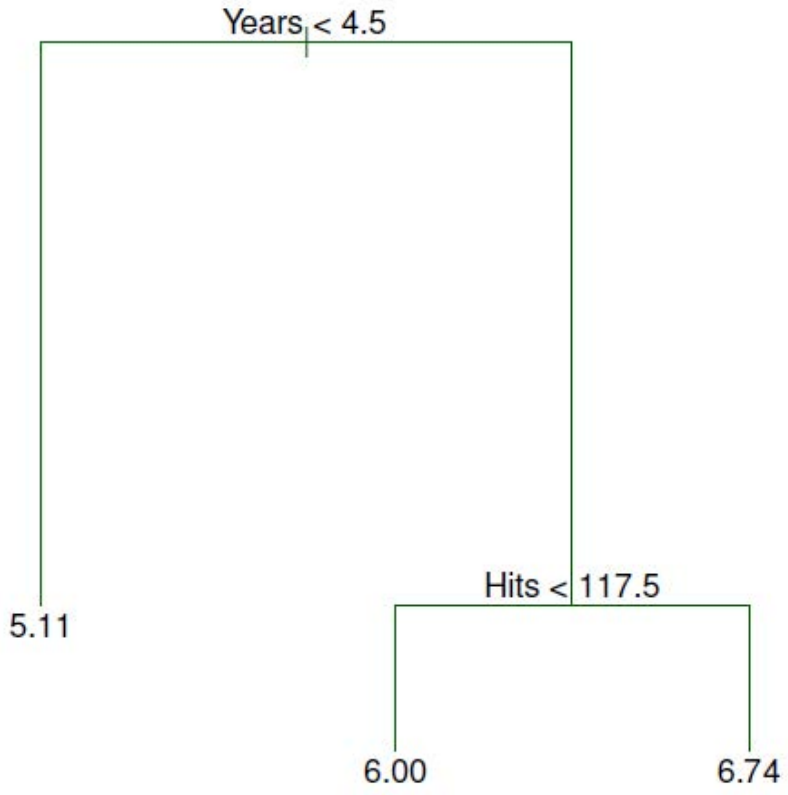

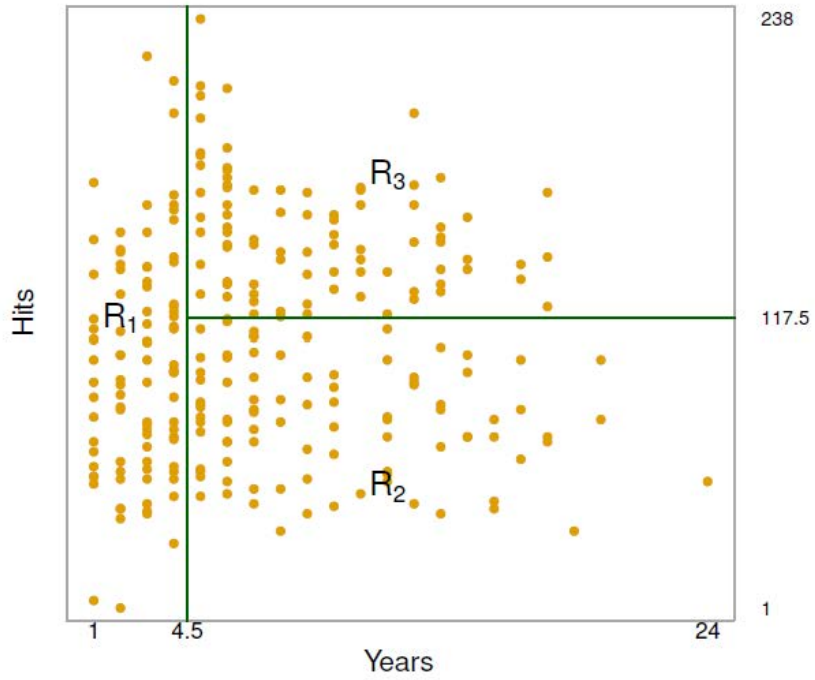

Classification Trees

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- If Y is categorical with K classes, then the class proportion $\hat{p} = \{\hat{p}_{mk}, m = 1, 2, \ldots, M \text{ and } k = 1, 2, \ldots, K\}$ could be found to be

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{i: x_i \in R_m} I(y_i = k)$$

and

$$k(m) = argmax_k \, \hat{p}_{mk}$$

- They are found by minimizing objective functions that include different measures of impurity $Q_m(T)$
  1. Misclassification error: $\frac{1}{N_m} \sum_{i: x_i \in R_m} I(y_i \neq k) = 1 - max_k \hat{p}_{mk}$
  2. Gini index (total variance): $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$ as a measure of purity which is small if the mth node is pure.
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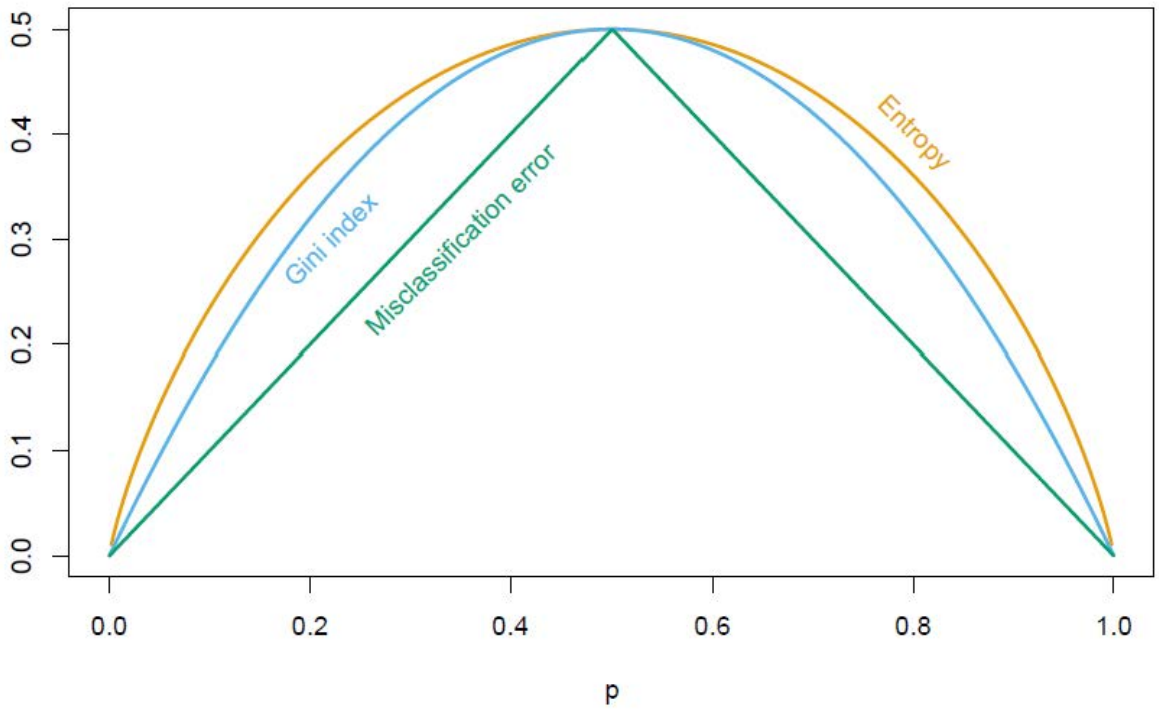
Classification Trees

Two class impurity functions with scaled cross-entropy function to go through (.5, .5)



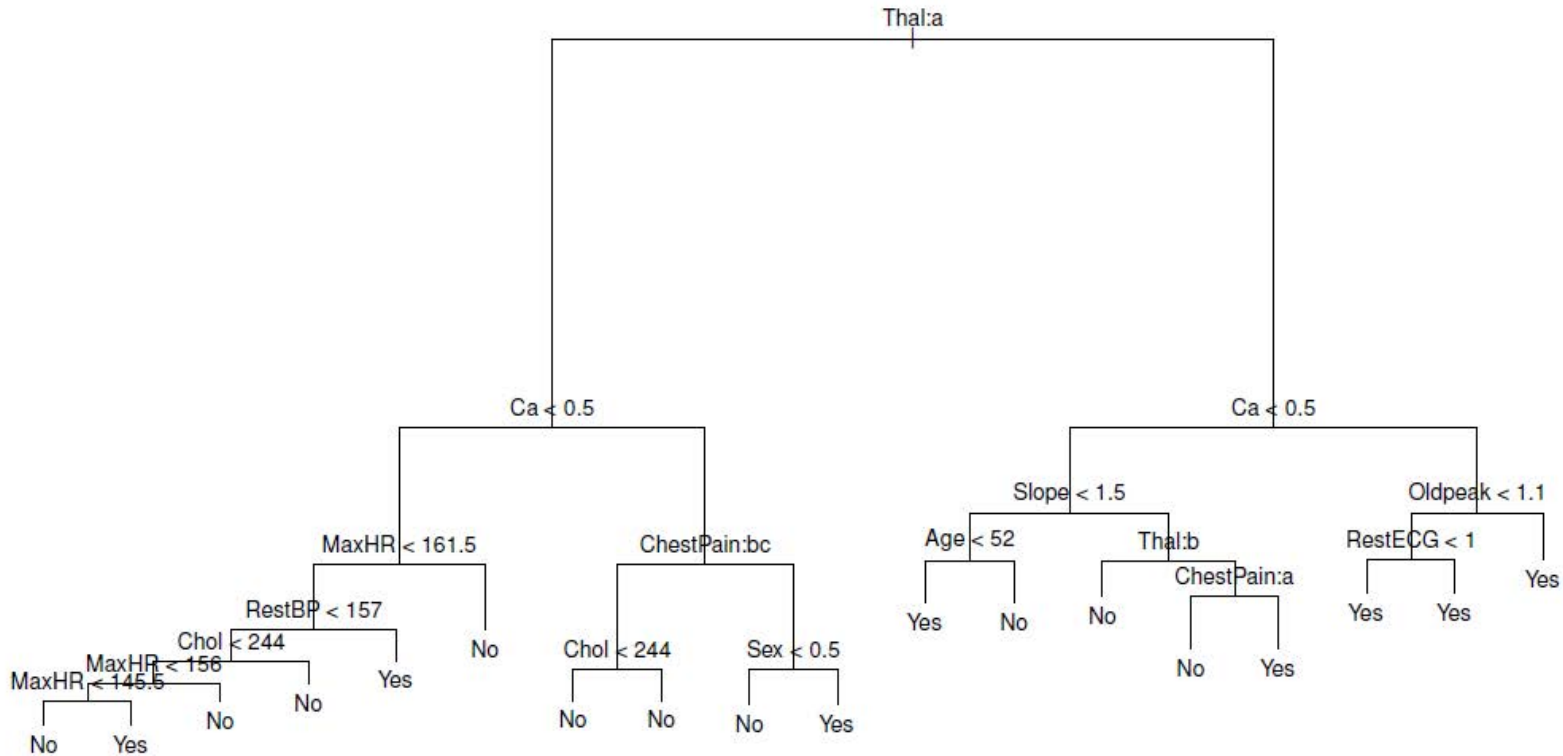
The functions are

1. Misclassification error: $1 - max(p, 1 - p)$
2. Gini index (total variance): $2p(1 - p)$
3. Cross-entropy (deviance): $-p \log(p) - (1 - p) \log(1 - p)$

Classification Trees

Example (Another Heart data)

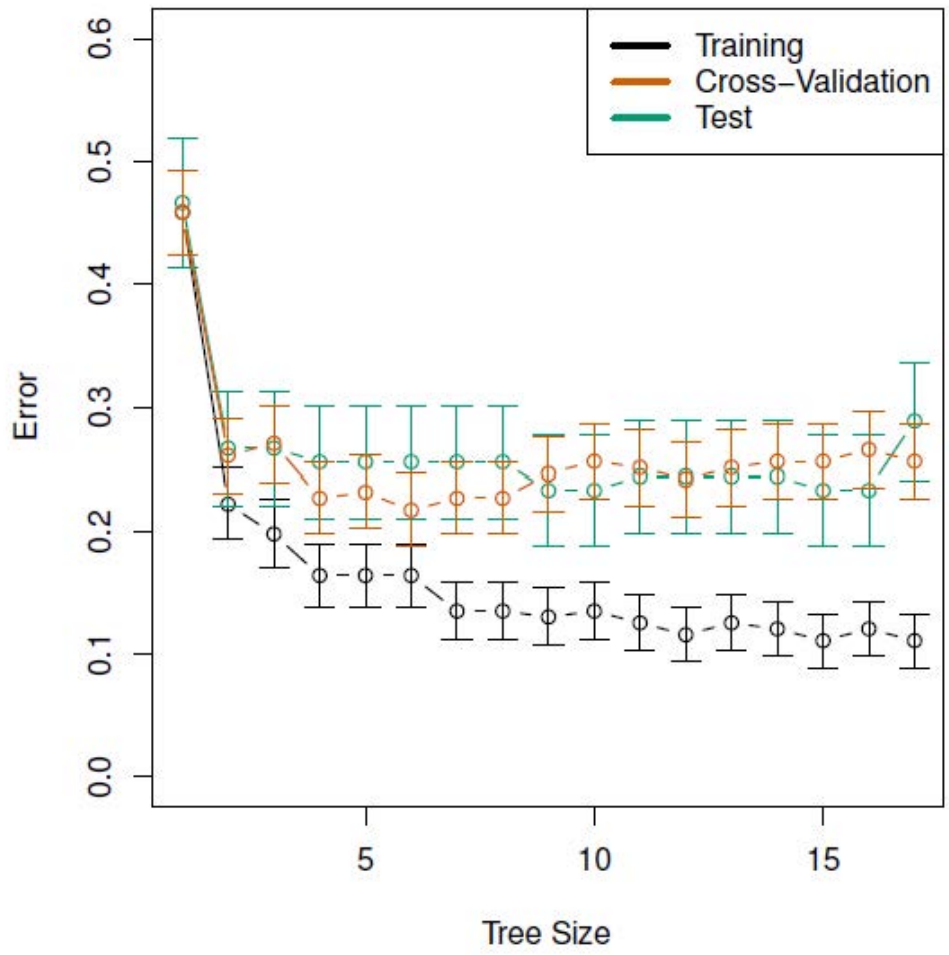
To predict heart disease HD (Y =Yes or No) based on 13 predictors Age, Sex, Chol, Thal,ChestPain, etc., CT gives T_0



Classification Trees

Example (Another Heart data)

A cross-validation will find the optimal tree size $|T| = 6$ (number of terminal nodes.)



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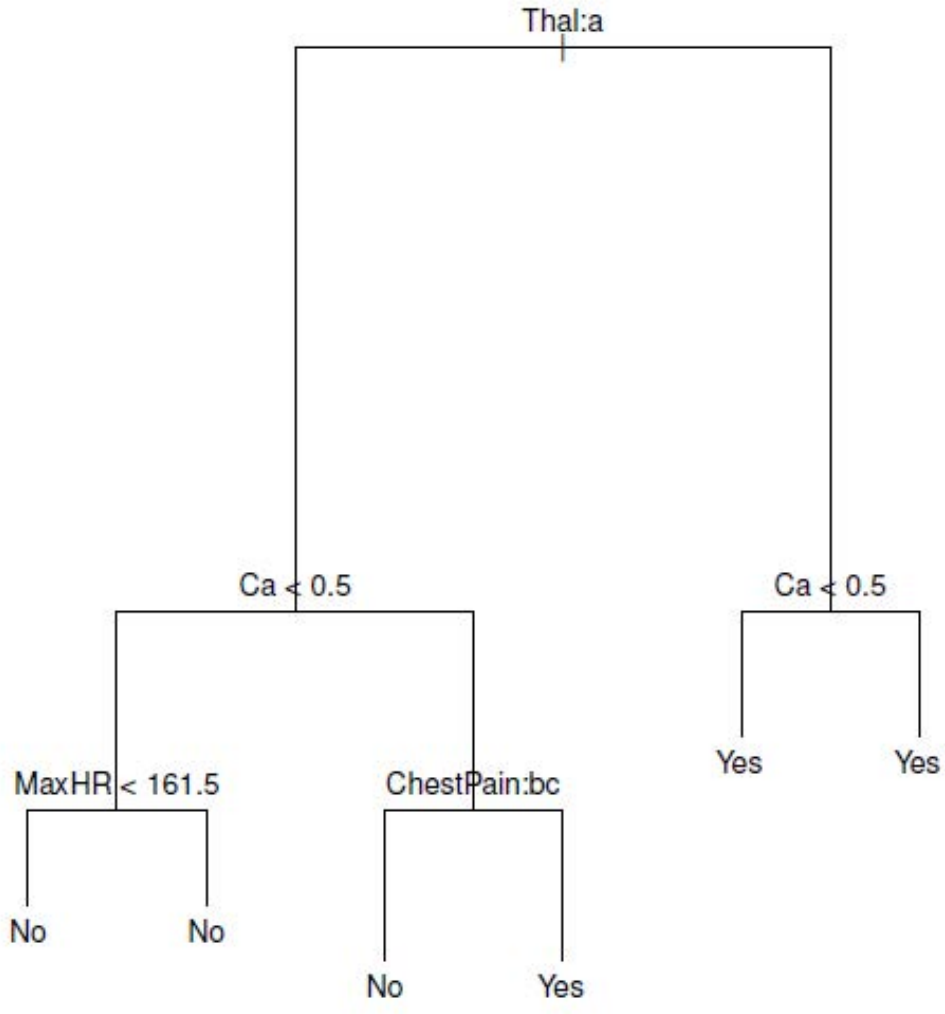
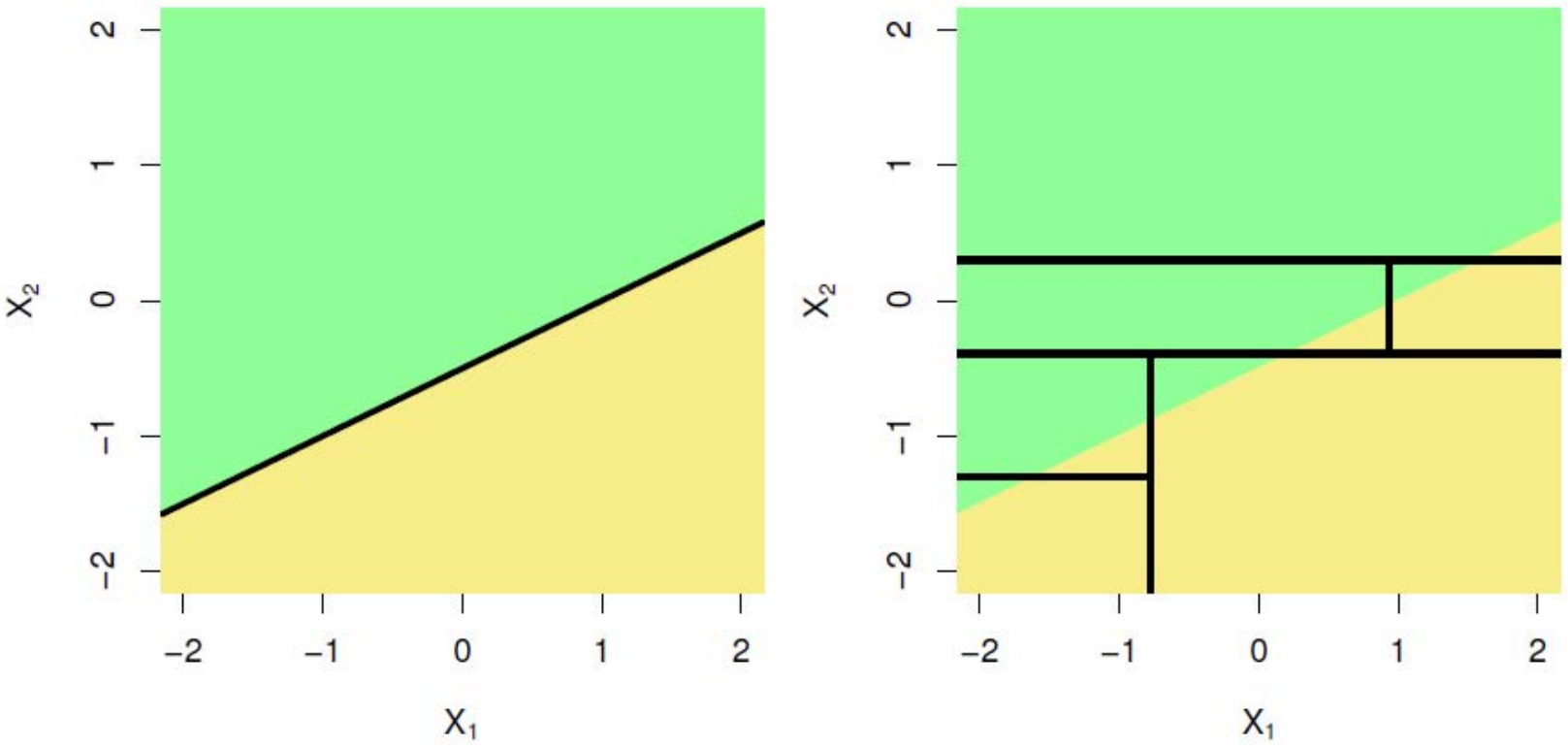


Tree-based methods vs. Linear models

Tree-based Methods

True linear decision boundary



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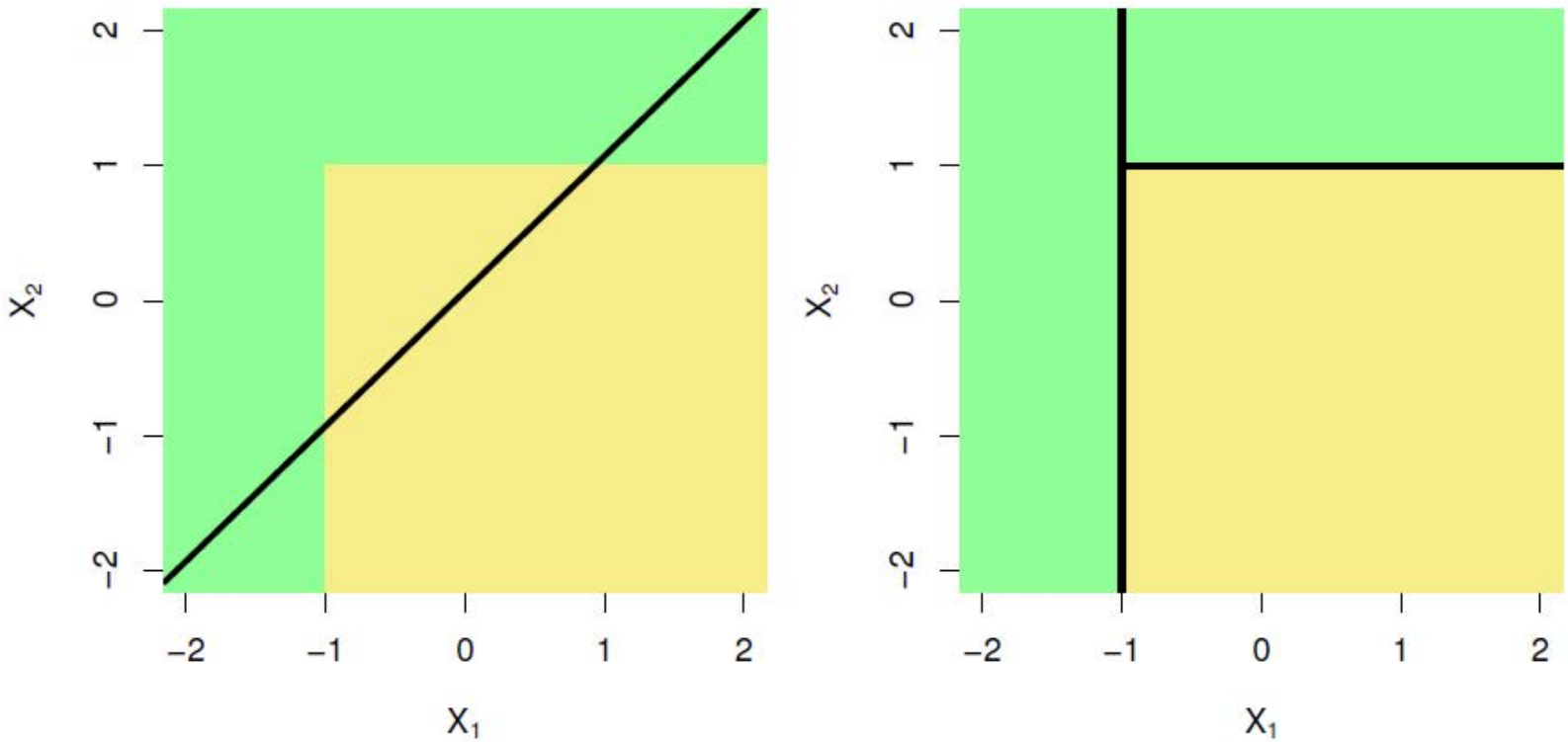

Tree-based Methods

Trees

- ⇑ easy to interpret
- ⇑ visually re-presentable
- ⇑ seem to resemble human decision making
- ⇑ handle categorical variables without dummy variables
- ⇓ less predictive accuracy
- ⇓ sensitive to slight changes in the data (not robust)

Tree-based Methods

DIY in R

1. Carry out a regression tree for the prostate cancer data using library(tree)
2. Carry out a classification tree for the SA hearth disease data using library(tree)

Please study the different methods in the ISL book.

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Please study the different methods in the ISL book.

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Hierarchical Mixtures of Experts (HME)

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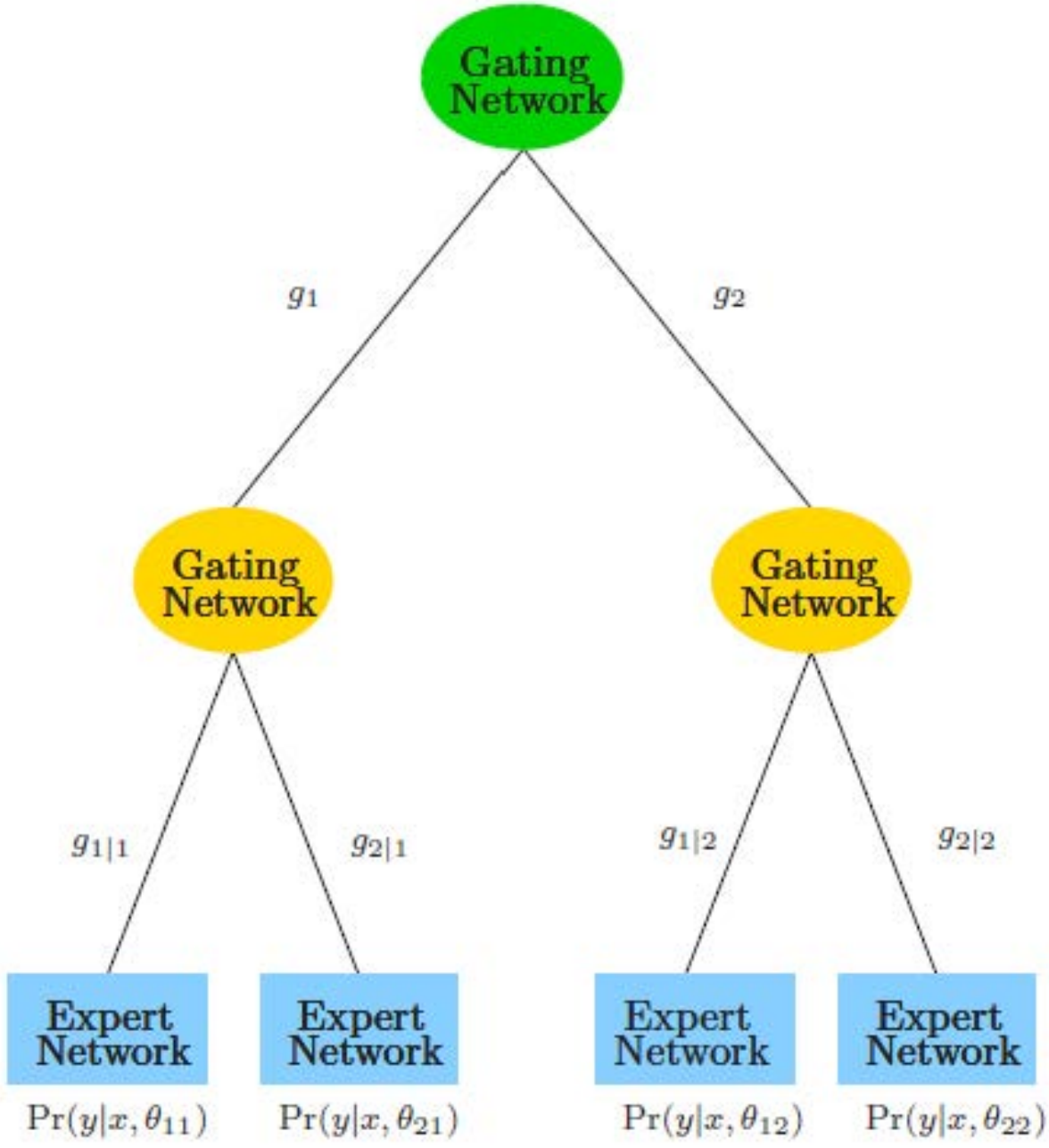

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- where $g_j(x, \gamma_j)$ is a softmax function in x with parameters γ_j
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- at the terminal the output $Y \sim P(y|x, \theta_{j\ell})$
  - Regression: P is normal with its parameters
  - Classification: P is the logistic CDF
- Then the mixture probability of the output is

$$P(y|x, \Psi) = \sum_{j=1}^{K} g_j(x, \gamma_j) \sum_{\ell=1}^{K} g_{\ell|j}(x, \gamma_{j\ell}) P(y|x, \theta_{j\ell})$$

- where $\Psi = (\gamma_j, \gamma_{j\ell}, \theta_{j\ell})$ is estimated using maximum likelihood methods and EM algorithm.

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End of Set 6