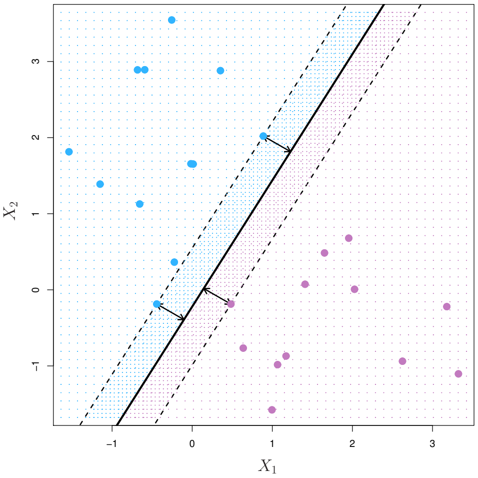
Decision Trees

Boosting and bagging

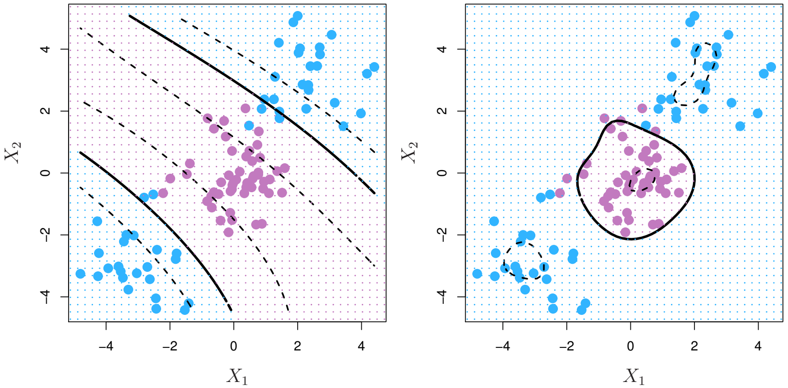
CS780/880 Introduction to Machine Learning

04/06/2017

SVM: Classification with Maximum Margin Hyperplane



Kernel SVM: Polynomial and Radial Kernels



Regression Methods

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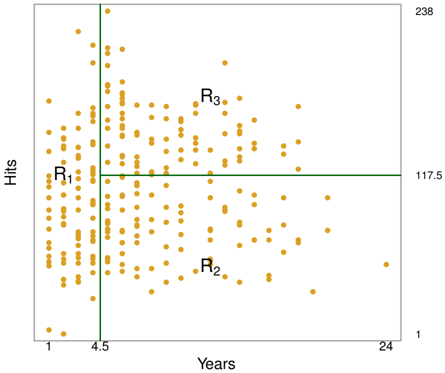
- Which ones are generative/discriminative?

Regression Trees

- Predict Baseball Salary based on Years played and Hits
- Example:

Tree Partition Space



Advantages/Disadvantages of Decision Trees

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  - Interpretability
  - Non-linearity
  - Little data preparation, scale invariance
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- Advantages:
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  - Little data preparation, scale invariance
  - Works with qualitative and quantitative features
- Disadvantages:
  - Hard to encode prior knowledge
  - Difficult to fit
  - Limited generalization

Decision Tree Terminology

- Internal nodes
- Branches
- Leaves

Types of Decision Trees

- Regression trees
- Classification tree

Learning a Decision Tree

- NP Hard problem

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- Approximate algorithms (heuristics):
  - ID3, C4.5, C5.0 (classification)
  - CART (classification and regression trees)
  - MARS (regression trees)
  - …

CART: Learning Regression Trees

Two basic steps:

1. Divide predictor space into regions $R_1, \ldots, R_J$

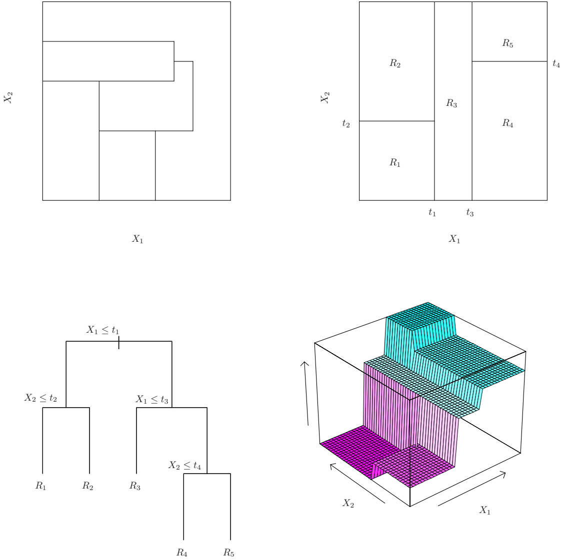
2. Make the same prediction for all data points that fall in R_j

CART: Recursive Binary Splitting

- Greedy top-to-bottom approach
- Recursively divide regions to minimize RSS

$$\sum_{x_i \in R_1} (y_i - \bar{y}_1)^2 + \sum_{x_i \in R_2} (y_i - \bar{y}_2)^2$$

CART: Splitting Example



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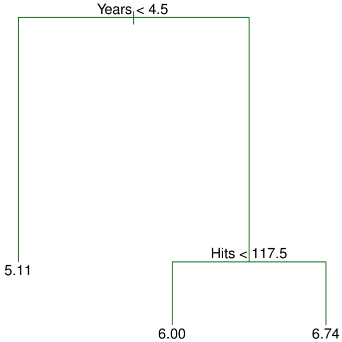
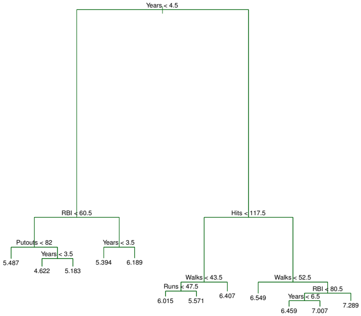
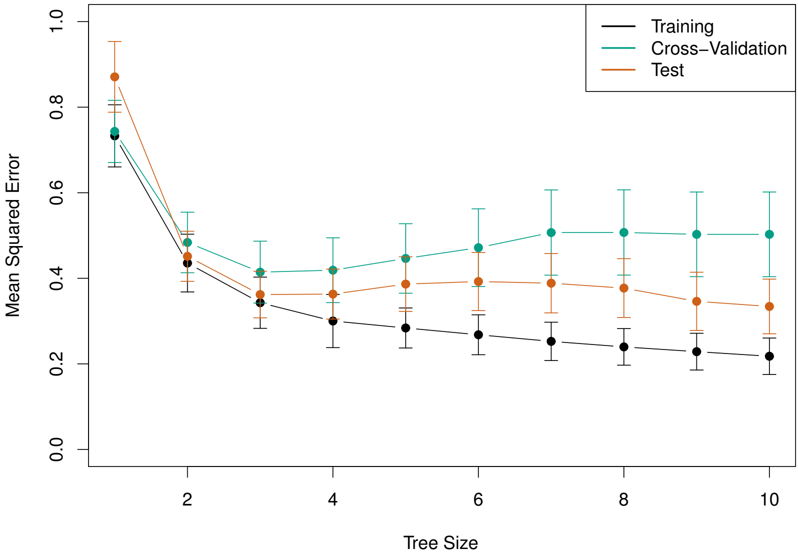
- Why is it better to prune than to stop early?

Pruning Example





Impact of Pruning

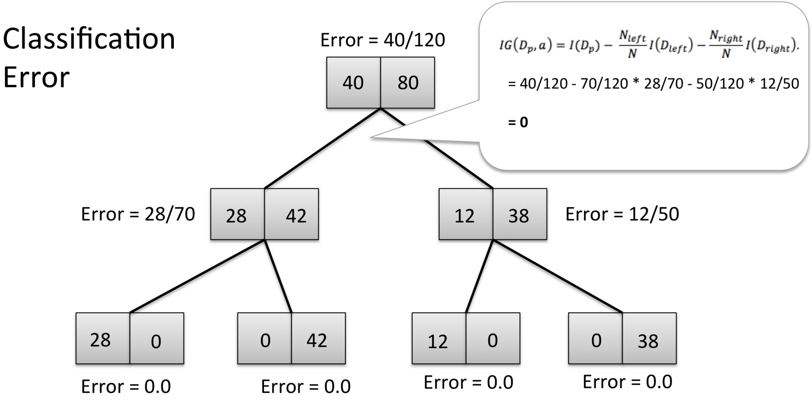


Classification Trees

- Similar to regression trees
- Except RSS does not make sense
- Use other measures of quality:
  1. Classification error rate
     $$1 - \max_k p_{mk}$$
     Often too pessimistic in practice
  2. Gini (impurity) index (CART):
     $$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{m_k})$$
  3. Cross-entropy (information gain) (ID3, C4.5):
     $$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{m_k}$$
- ID3, C4.5 do not prune

Why Not Use Classification Error?

Decision tree with classification error



Source: `https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html`

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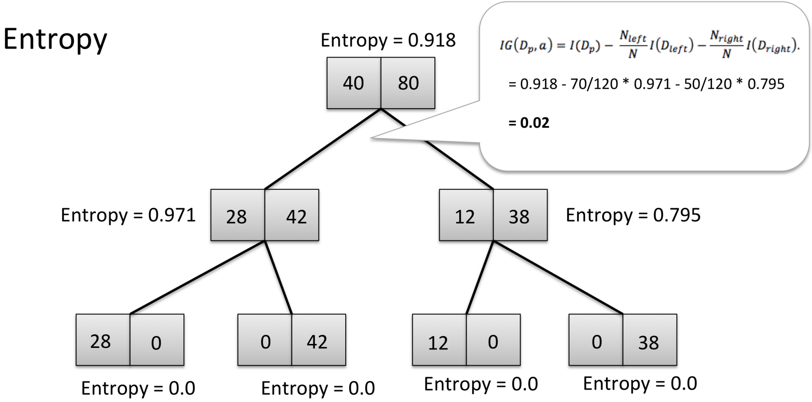

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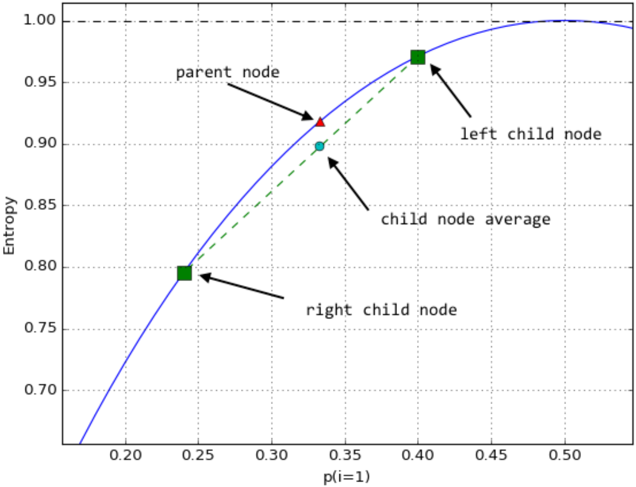
Why Not Use Classification Error?

Entropy is more optimistic



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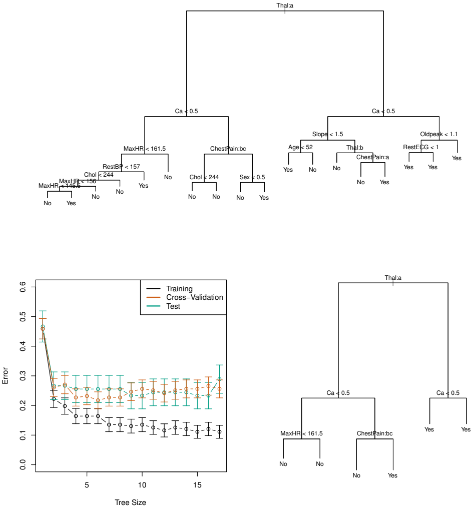
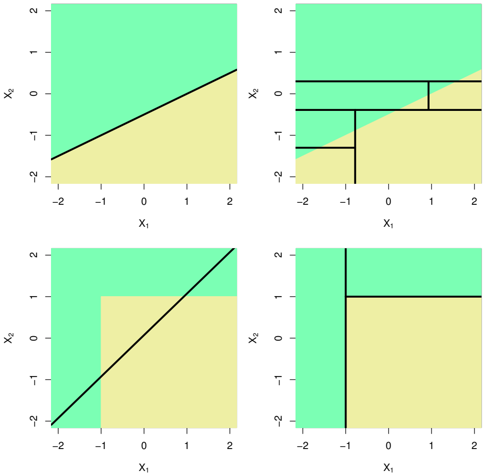
Pruning in Classification Trees



Trees vs. Linear Models



Trees vs. KNN

Trees vs. KNN

- Trees do not require a distance metric
- Trees work well with categorical predictors
- Trees work well in large dimensions
- KNN are better in low-dimensional problems with complex decision boundaries

Bagging and Boosting

- Methods for reducing variance of decision trees
- Make predictions using a *weighted vote* of multiple trees
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- Disadvantage of using votes of multiple trees?

Bagging

- Stands for "Bootstrap Aggregating"
- Construct multiple bootstrapped training sets:

$$T_1, T_2, \ldots, T_B$$

- Fit a tree to each one:

$$\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_B$$

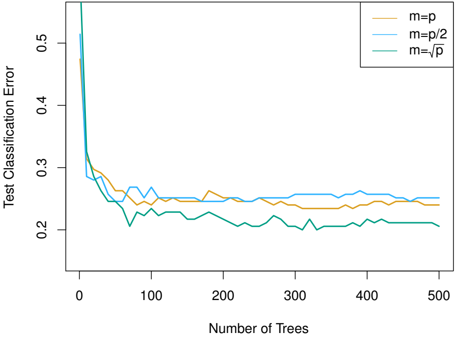
- Make predictions by averaging individual tree predictions

$$\hat{f}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b(x)$$

- Large values of B are not likely to overfit, $B \approx 100$ is a good choice

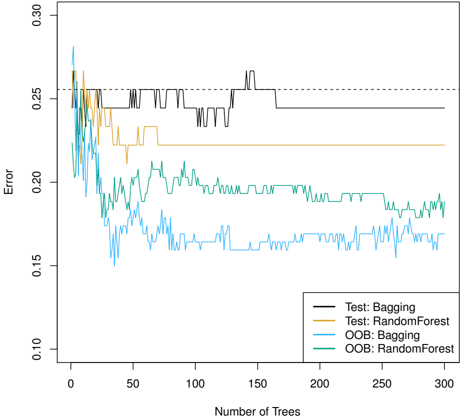
Random Forests

- Many trees in bagging will be similar
- Algorithms choose the same features to split on
- Random forests help to address similarity:
  - At each split, choose only from m randomly sampled features
- Good empirical choice is $m = \sqrt{p}$



Cross-validation and Bagging

- No need for cross-validation when bagging
- Evaluating trees on out-of bag samples is sufficient



Boosting (Gradient Boosting, AdaBoost)

What Kaggle has to say:

source:

http://blog.kaggle.com/2017/01/23/a-kaggle-master-explains-gradient-boosting/

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- Assume we have $1 \ldots m$ trees and weights, next best tree?

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- Compute the weight λ by **line search**
- And many other bells and whistles

XGBoost

- Scalable and flexible gradient boosting
- Interfaces for many languages and environments