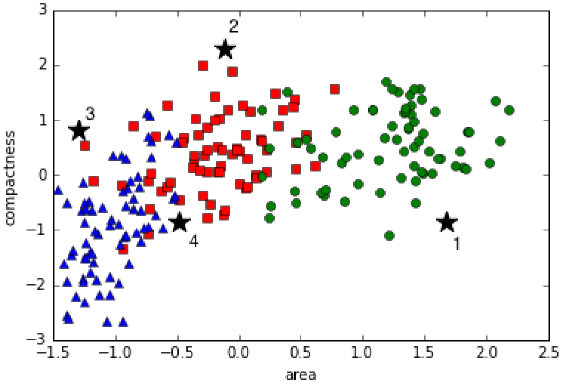
Lecture 11 – KNN and Decision Trees

ECE 597ML-697ML

Mario Parente

Nearest Neighbor Classification

Seed classification by area and compactness



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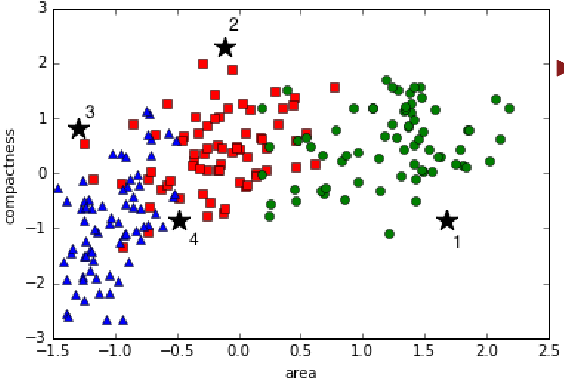

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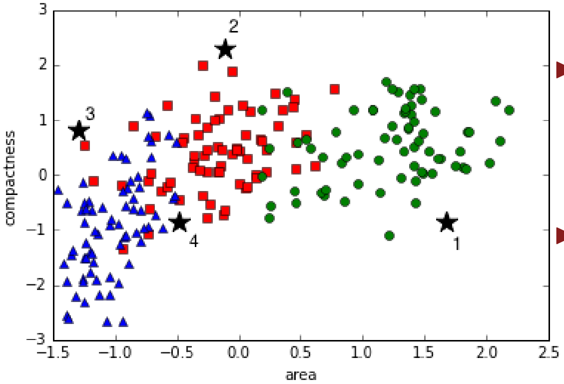

- What should we predict for unlabeled test points (stars)?
- Nearest neighbor classification: predict label of nearest training example
- k-nearest neighbor: predict consensus of k nearest training examples

k-Nearest Neighbor Classification

- **Training**: store the training data (trivial!)

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- KNN can work with any distance function and any value of k. We need to choose these.

Distance and Similarity

- KNN can use any **distance function** to determine k nearest neighbors. A distance function $d(\mathbf{x}, \mathbf{x}')$ takes two data points and returns a distance. It should satisfy
  - $d(\mathbf{x}, \mathbf{x}') \geq 0$ (non-negativity)
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- Or you can use a *similarity function*
  - $s(\mathbf{x}, \mathbf{x}') \geq 0$
  - $s(\mathbf{x}, \mathbf{x}) \geq s(\mathbf{x}, \mathbf{x}')$ for all other $\mathbf{x}'$ ($\mathbf{x}$ is more similar to itself than any other point)

Euclidean Distance

- We've already seen one distance function, the **Euclidean distance**:

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Minkowski Distance

- A more general class of distance functions come from **Minkowski Distance**

$$d_p(\mathbf{x}, \mathbf{x}') := \|\mathbf{x} - \mathbf{x}'\|_p$$
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  - $p = 2$ is Euclidean distance (verify on own)
  - $p = 1$ is called the "Manhattan distance", intutition (2D): path "around the block"
  - $p = \infty$ is called the Chebyshev's distance $d_\infty(\mathbf{x}, \mathbf{x}') \max_i(|x_i - x_i'|)$, intutition (2D): In a warehouse, the distance between locations can be represented as Chebyshev distance if an overhead crane is used because the crane moves on both axes at the same time with the same speed.

Examples

- Jupyter Demo 1: different distance functions

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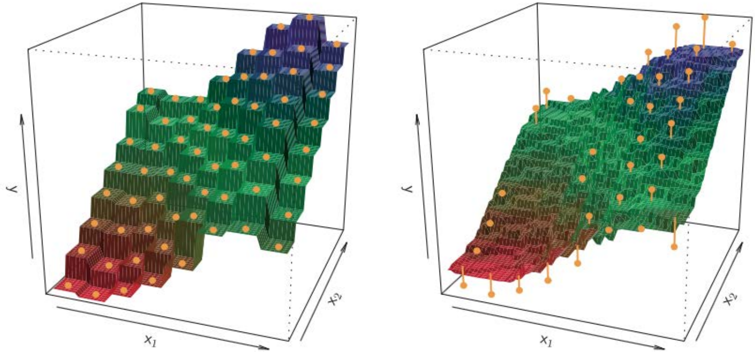
- In practice, clever data structures (e.g., KD-trees) can be constructed to find k nearest neighbors and make predictions more quickly.

KNN regression

- The KNN regression is a non-parametric regression method that simply stores the training data D and makes a prediction for each new instance $\mathbf{x}$ using an average over its set of K nearest neighbors $\mathcal{N}_K(\mathbf{x})$ computed using any distance function d as in classification.

$$f_{KNN}(\mathbf{x}) = \frac{1}{K} \sum_{i \in \mathcal{N}_K(\mathbf{x})} y^{(i)}$$

Example: 2D KNN regression (K=1, and K=9)



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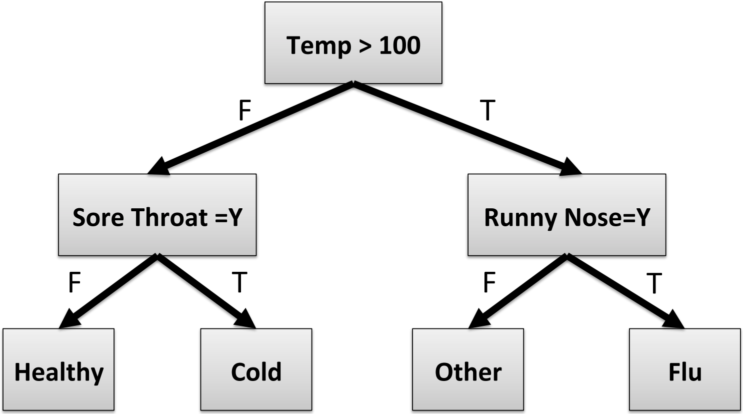
- Jupyter Demo 2: KNN in action
  - Effect of k
  - KNN convergence as data goes to infinity

Decision Trees

Example: Flu decision tree



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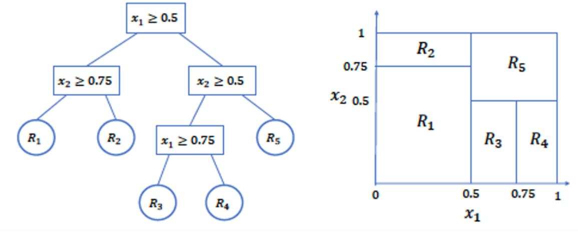
  - Leaf nodes are assigned labels $\rightarrow$ prediction for $\mathbf{x}$

Regression Trees



$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m I(\mathbf{x} \in R_m)$$

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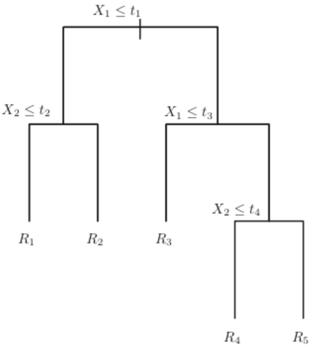

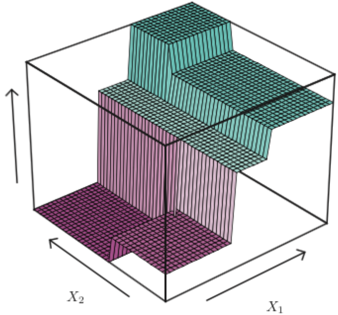

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- How do we find best splits? Exhaustive search: NP-hard. Need greedy algorithm

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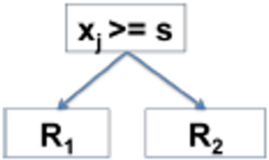

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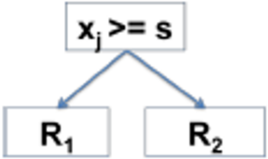

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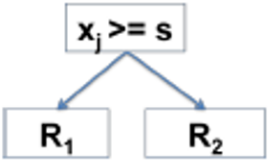

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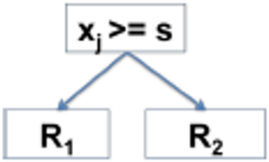

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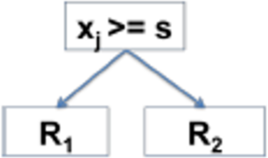

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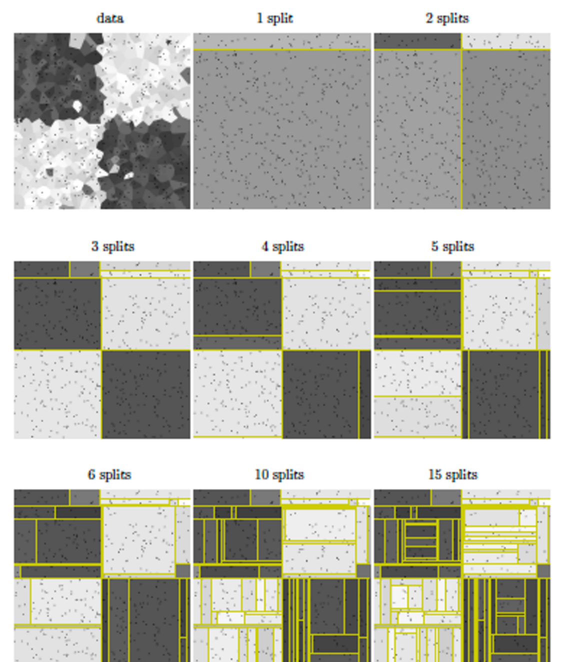
- Split the data based on where it falls
- Recurse on each branch
- Stop eventually (to control capacity of the tree) at maximum depth, at maximum number of terminal nodes, at maximum number of splits (and many others)

Regression Tree Learning: Examples



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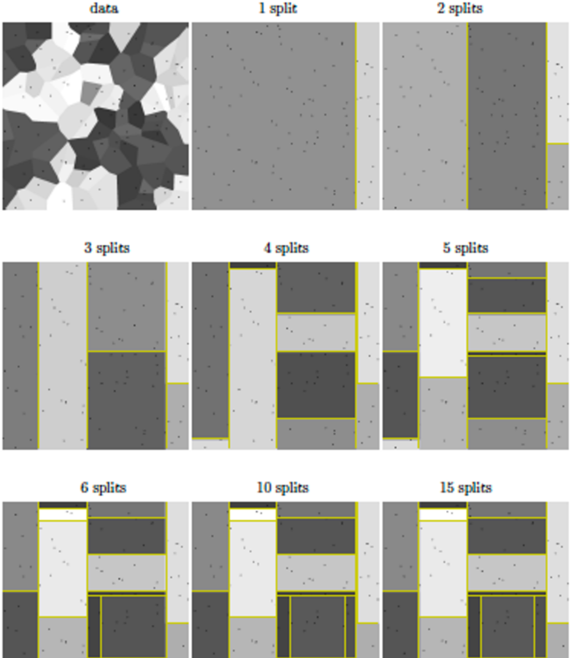


Complexity

The runtime of a naive implementation is pN^2 where p number of dimensions and N number of training points. We can improve this by using recursive algorithms which brings the run time to $pN \log N$.

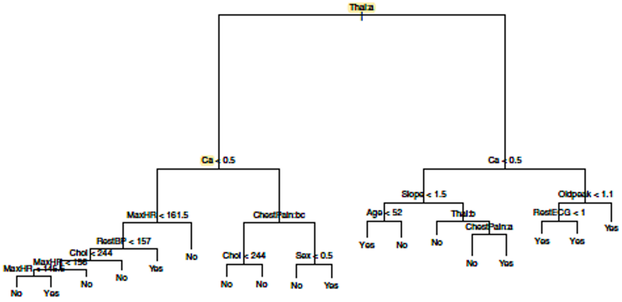
Tree Pruning

- training procedure: grow a tree up to a certain depth D. Could lead to overfitting (high complexity, low bias, high variance)
- instead of stopping early, grow large tree T_0 and prune later using complexity pruning (or weakest link pruning)

$$\sum_{m=1}^{|T|} \sum_{\mathbf{x}^{(i)} \in R_m} (y^{(i)} - \hat{y}_{R_m})^2 + \alpha |T|$$

  (first term is training error, secind penalty on number of leaves)
- cross-validate α

Classification Trees



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- How do we find best splits? We use recursive binary splitting but can't use MSE as cost.
- First, we write the fraction of training data in region m with label k to be

$$\hat{P}_{mk} = \frac{1}{N_m} \sum_{\mathbf{x}^{(i)} \in R_m} I(y^{(i)} = k)$$

Our intuition is to let $\hat{P_{mk}}$ have low randomness.

Classification Tree Learning

We have the following choices to measure randomness.

- Misclassification Error $1 - \max_k \hat{P_{mk}}$. This is rarely used since it not sufficiently sensitive for tree growing.

- Gini Index

$$\sum_{k=1}^{K} \sum_{k \neq k'} \hat{P_{mk}} \hat{P_{mk'}} = \sum_{k=1}^{K} \hat{P_{mk}} \left(1 - \hat{P_{mk}}\right)$$

- Cross Entropy (from information theory)

$$-\sum_{k=1}^{K} \hat{P_{mk}} \log \hat{P_{mk}}$$

One can show that the entropy will take on a value near zero if the $\hat{P_{mk}}$ are all near zero or near one. In practice, Gini Index and Cross Entropy usually have similar effects.

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  - **Accuracy** By themselves, not always as performing as NN or SVM.
- General advice: decision trees are very competitive "out-of-the-box" machine learning models for lots of problems if associated with methods such as bagging, random forests or boosting.

Bagging for Trees

- Trees have high veriance (if fit a tree to two halves of training set can get different results)
- If one can extract several training sets from population and average predictions (regression) or take majority vote (classification) over each set can lower variance
- We only have one dataset: bootstrap (select several training samples with replacement) and average predictions (regression) or take majority vote (classification). This is called bagging.
- in bagging the trees are grown deep and not pruned (low bias, high variance)
- B larger is better but higher computational complexity and diminishing returns in accuracy the larger it is.

Out-of-Bag Error Estimation

- No need for crossvalidation to estimate test error of bagged model. Each bootstrapped tree makes use of around two thirds of the observations. Can use the rest (out-of-bag or OOB) observations for testing
- single observation $\mathbf{x}$ is OOB for around $B/3$ trees (B is the $\#$ of trees created by bootstrapping). Predict output for $\mathbf{x}$ for each tree and average (regression) or majority vote (classification).

Variable Importance

- Total amount that the MSE (regression) or the Gini Index (classification) is decreased due to splits over a given predictor, averaged over all B trees. A large value indicates an important predictor.
- One can train the ensamble only using the l most important features. Slight decrease in performance but boost in computation time gain.

Random Forests

As in bagging, we build a number of decision trees on bootstrapped training samples. But when building these decision trees, each time a split in a tree is considered, a random sample of m predictors is chosen as split candidates from the full set of p predictors. The split is allowed to use only one of those m predictors. A fresh sample of m predictors is taken at each split, and typically we choose $m = \sqrt(p)$ but can cross-validate over m.

This avoids having that all trees use particularly strong predictors in the top split, making the trees correlated.

Low value of m preferrable when we have large number of correlated predictors.