INFO 251: Applied Machine Learning

Random Forests

Thanks to machine-learning algorithms,
the robot apocalypse was short-lived.

Key Concepts (Decision Trees)

- Churn prediction
- Decision tree representation
- Hyper-rectangles and decision boundary
- Recursive tree building algorithm
- Splitting
- Information gain

Intuition check

- True or false:
  - The recursive decision tree algorithm is deterministic (assuming we are not performing cross-validation and have fixed the hyperparameters in advance)

Course Outline

- Causal Inference and Research Design
  - Experimental methods
  - Non-experiment methods
- **Machine Learning**
  - Design of Machine Learning Experiments
  - Linear Models and Gradient Descent
  - Fairness and Bias in ML
  - **Non-linear models**
  - Neural models
  - Deep Learning
  - Practicalities
  - Unsupervised Learning
- Special topics

Outline

- Regression Trees
- Random Forests
- Ensembles
- Boosting
- Feature Importance

Key Concepts (Random Forests)

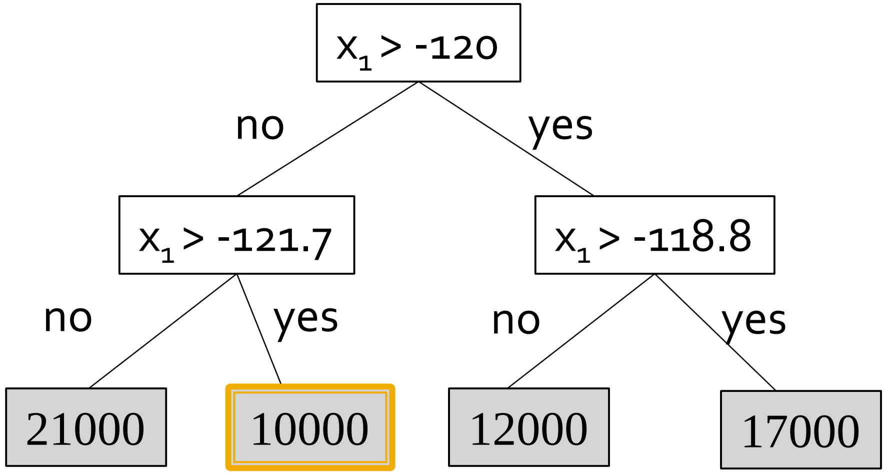
- Regression vs. Decision trees
- Recursive regression trees algorithm
- Random forests
- Bagging
- Stacking
- Adaboost
- Gradient boosting
- Feature importance

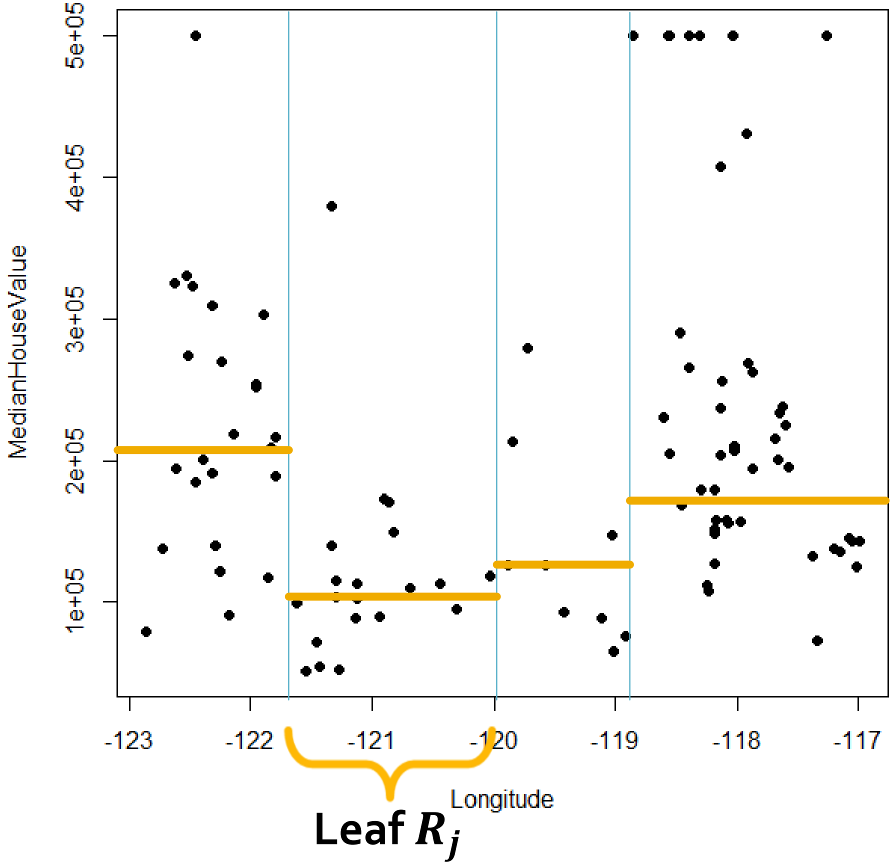
Regression Trees

- What if output values are continuous or real-valued (i.e., not discrete)?
- Regression trees
  - Construct binary tree, minimize error in each leaf
  - Before, we counted # elements of each type in leaf
  - Now we choose predicted value that minimizes error
- Example: Predict median housing value based on a house's location (latitude, longitude)

Regression Trees

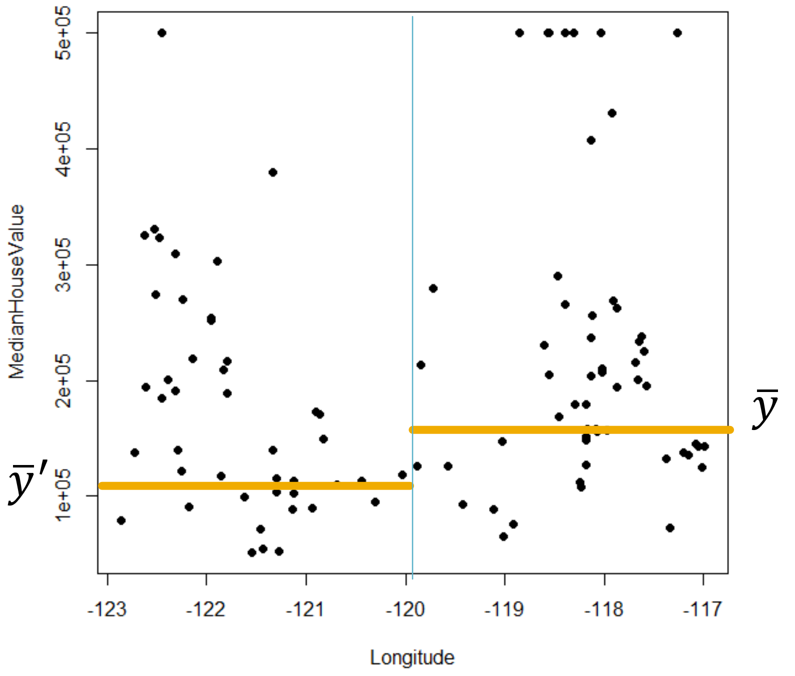
```
> head(calif[,c(1,8,9)])
  MedianHouseValue Latitude Longitude
1           452600    37.88   -122.23
2           358500    37.86   -122.22
3           352100    37.85   -122.24
4           341300    37.85   -122.25
5           342200    37.85   -122.25
6           269700    37.85   -122.25
                ...
```





Regression Trees

- How to choose split point?
  - Idea: Minimize prediction error
- In 1-dimension: choose *s* to minimize
  - $\min_{\bar{y}} \sum_{i:x_i>s} (\bar{y} - y_i)^2 + \min_{\bar{y}'} \sum_{i:x_i \le s} (\bar{y}' - y_i)^2$
  - Consider finite splits (e.g. *s* between data)
- This intuition generalizes to *D* dimensions

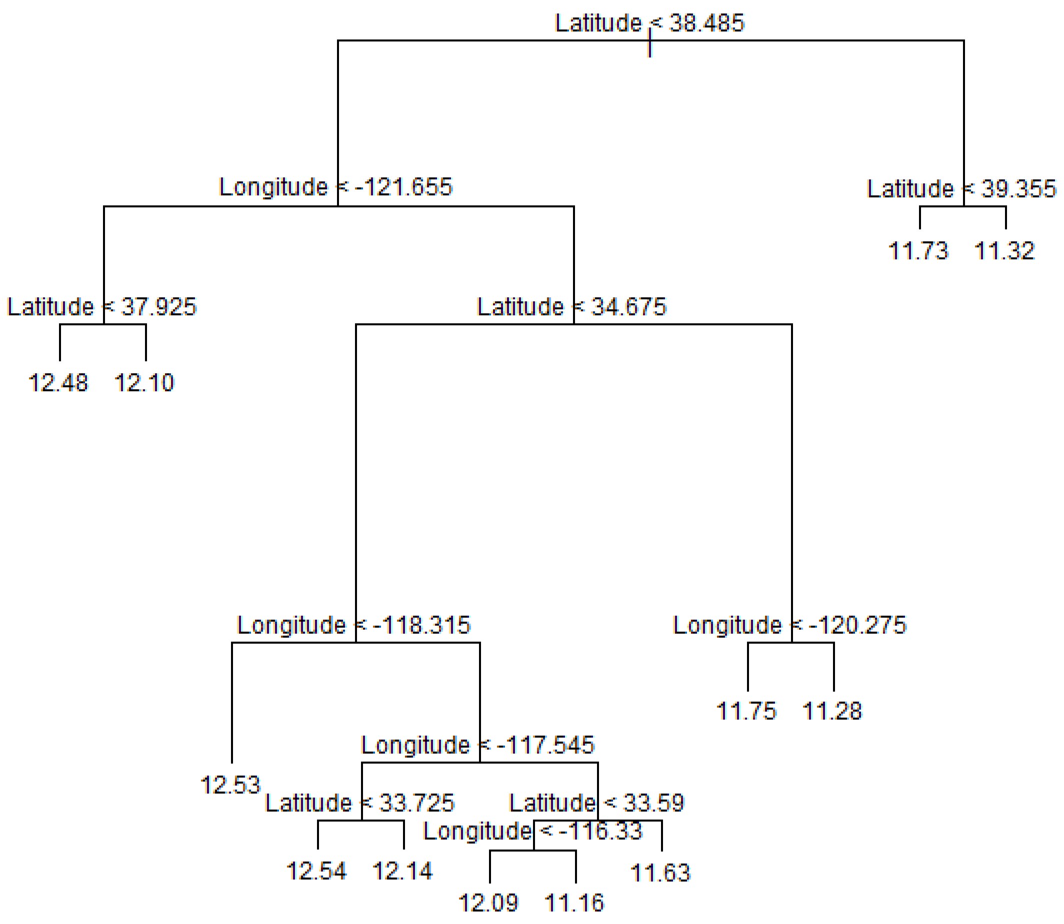


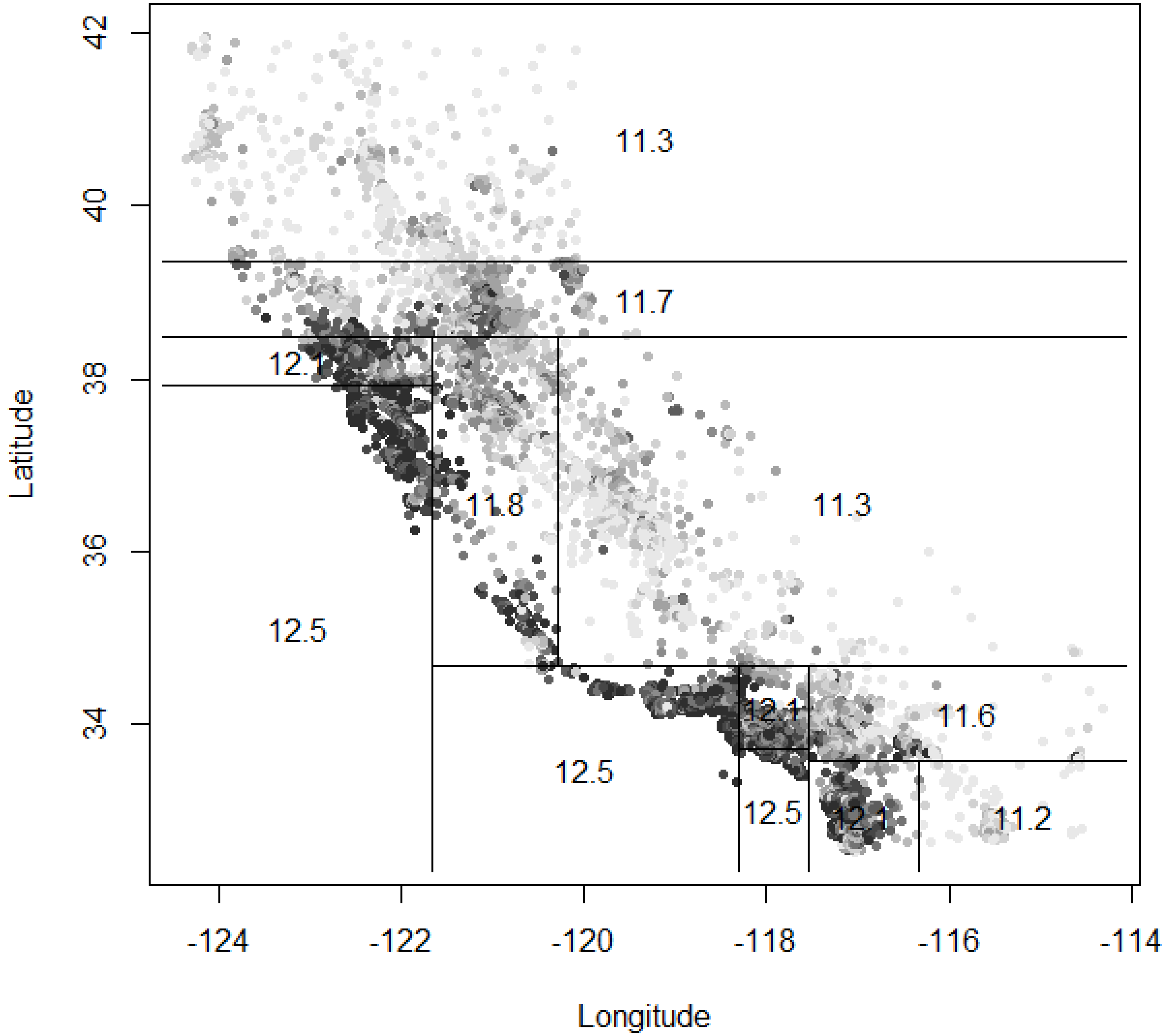
Regression Trees: Recursive Algorithm

1. Start with a single node (c_j) containing all points.
   1. Calculate predicted value $\bar{y}_{c_j} = \frac{1}{n} \sum_{i \in c_j} y_i$
   2. Calculate total error: $J = \sum_{c_j} \sum_{i \in c_j} \left(\bar{y}_{c_j} - y_i \right)^2$
2. If all points in the node have identical features (predictors), stop.
   - Otherwise, search all binary splits of all variables for split that most reduces J
   - Stop if J decreases less than δ or if nodes are close to empty
   - Otherwise, make that split, creating two new nodes
3. Recurse on each new node

See also: Chapter 9 (especially 9.2) of Elements of Statistical Learning

Regression Trees: Example





Outline

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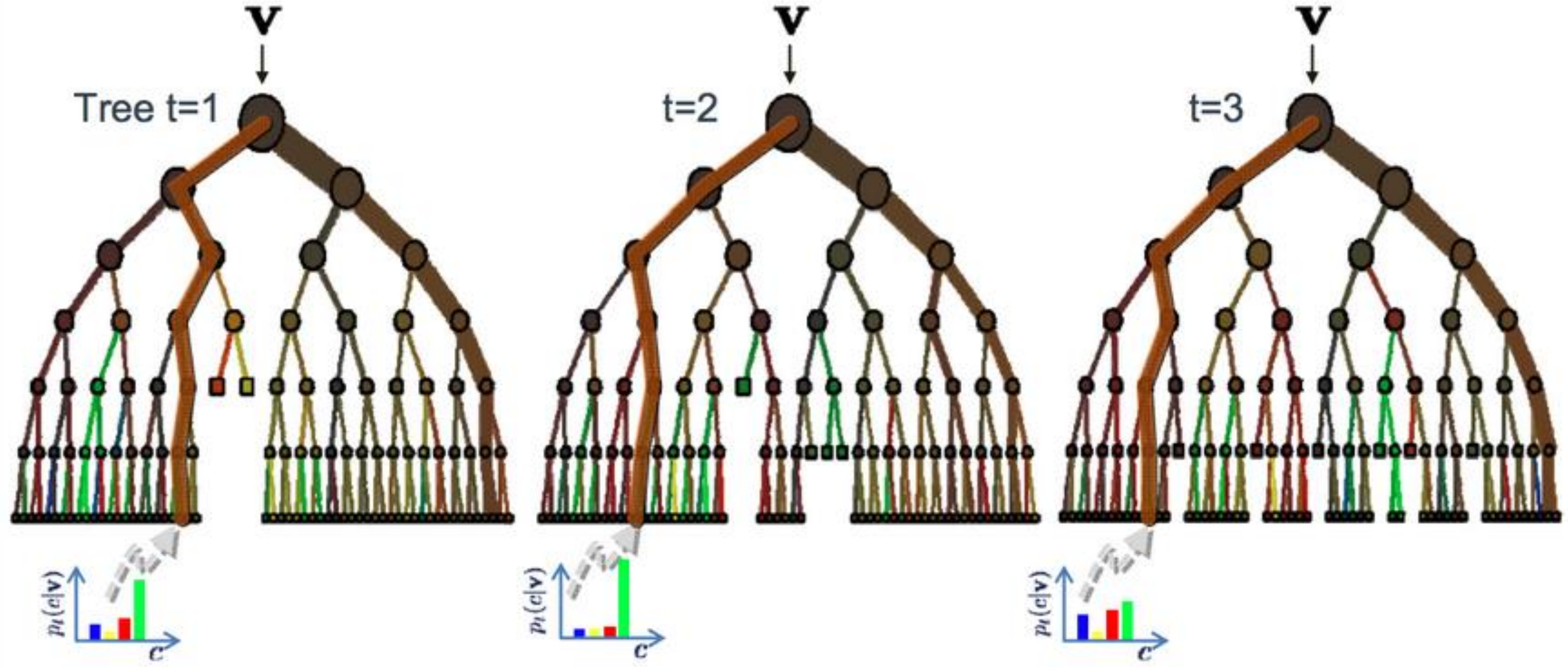
- **Random Forests**
- Ensembles
- Boosting
- Feature Importance

Trees to forests

- Which classifier works best?
  - "Random forests" combine outputs of multiple classifiers



Building a forest

- Bootstrap sample a new training set
  - with replacement
- Build a decision tree
  - The randomization (of the sample and/or features) forces differentiated trees
  - Optional: randomly select a subset of features
  - Pruning not required! “Regularization” occurs through forest
- Repeat until you have lots of trees
- Predict by taking a vote among the trees

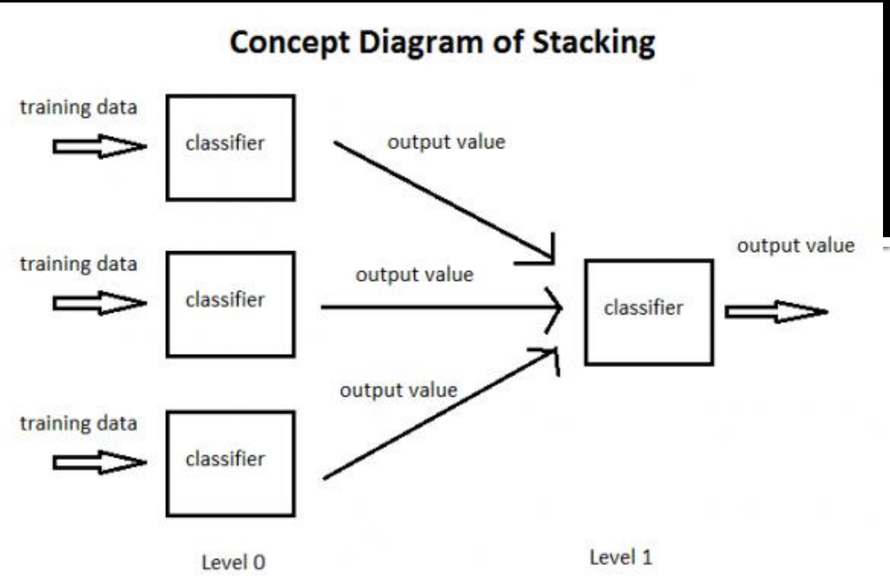
Example: The "CART" forest

- Formally:

$$\hat{y}_i = \sum_{f_k \in \mathcal{F}} f_k(x_i)$$

- $\mathcal{F}$ is the space of regression trees
  - Each f_k maps data examples x_i to tree leaves
  - Scores are averaged (or summed, depending on implementation) across trees

Other ensemble methods



- Bagging = **b**ootstrap **agg**regat**ing**
  - Create artificial versions of data via bootstrap
  - 1 sample = bootstrap
  - *M* samples = bagging
- Stacking: train model (e.g. another tree, a logistic regression) on output of other models
- Boosting (Kearns, 1988)
  - Train a sequence of models, each emphasizes the examples misclassified by the previous model

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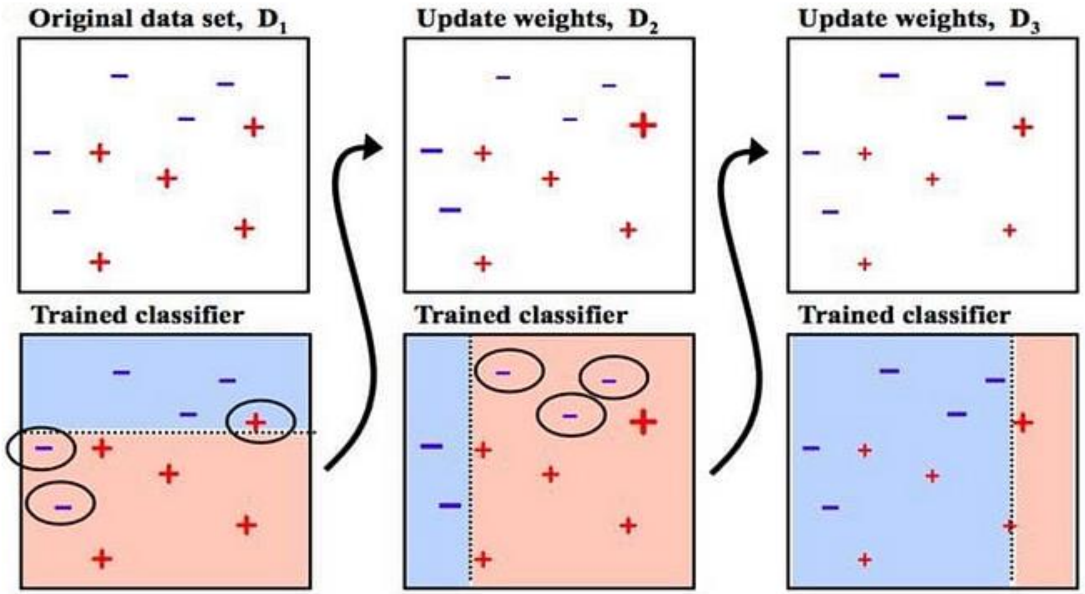
Adaptive Boosting (AdaBoost)

- Adaboost:

1. Initially, set a uniform weight for each training example = 1/n
2. Train a classifier where the objective respects the weights
   - Could be any classifier, but original Adaboost used single-feature decision stump
3. Increase the weights for misclassified examples
4. Return to 2



Bauer, E. and Kohavi, R. An empirical comparison of voting classification algorithms: Bagging, boosting and variants. *Machine Learning 36* (1999), 105–142.

Gradient Boosting

(Extreme) Gradient Boosting

- Start with regression tree-based model:

$$\hat{y}_i = \sum_{f_k \in \mathcal{F}} f_k(x_i)$$

- Gradient boosting loss function "fits on residuals":

$$\mathcal{L}^{(t)} = \sum_{i=1}^{n} l(y_i, \underbrace{\hat{y}_i^{(t-1)} + f_t(x_i))}_{f_t \text{ fits on residual of t-1}} + \underbrace{\gamma T + \frac{1}{2}\lambda \|w\|^2}_{\text{Regularization penalties}}$$

  - T is the number of leaves
  - t indexes training iterations
  - w is vector of scores on each leaf (i.e., the leaf weights)

- Optimization is similar to gradient descent
  - Relies on being able to measure how good each tree is
  - Next tree solves for the loss of prior tree

Details Friedman, J.H., 2001. Greedy function approximation: a gradient boosting machine. Annals of statistics 1189–1232.
See also: Chapter 10.9 and 10.10 of Elements of Statistical Learning

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- Regression Trees
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- **Feature Importance**

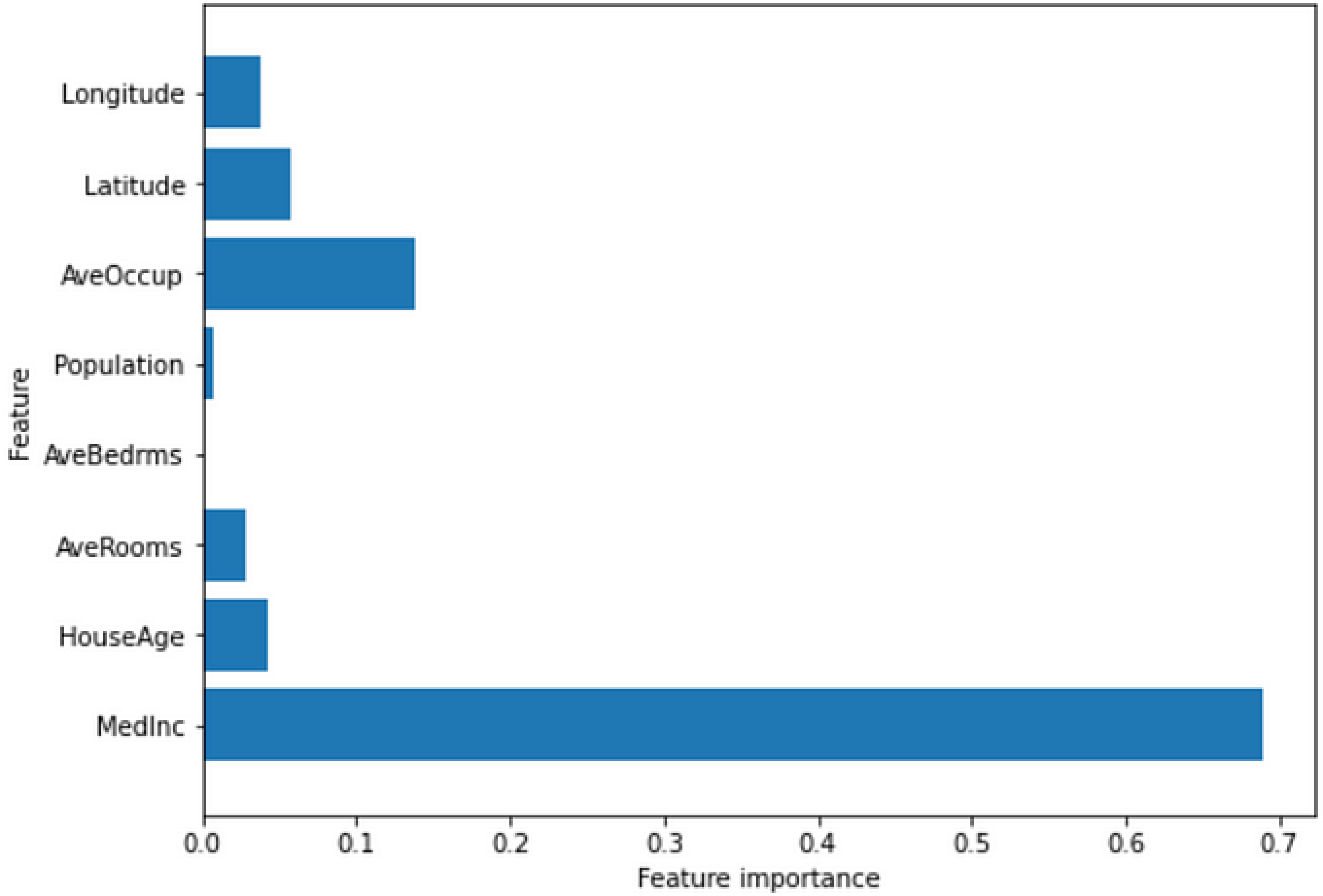
Feature Importance

- The primary focus of random forests is prediction, rather than inference
  - A single tree is fairly interpretable, but it's hard to interpret a forest
  - This is generally true for complex, non-parametric, and non-linear models
- Nonetheless, people frequently still want to do some ex-post interpretation
  - "What features are important to the classifier?"

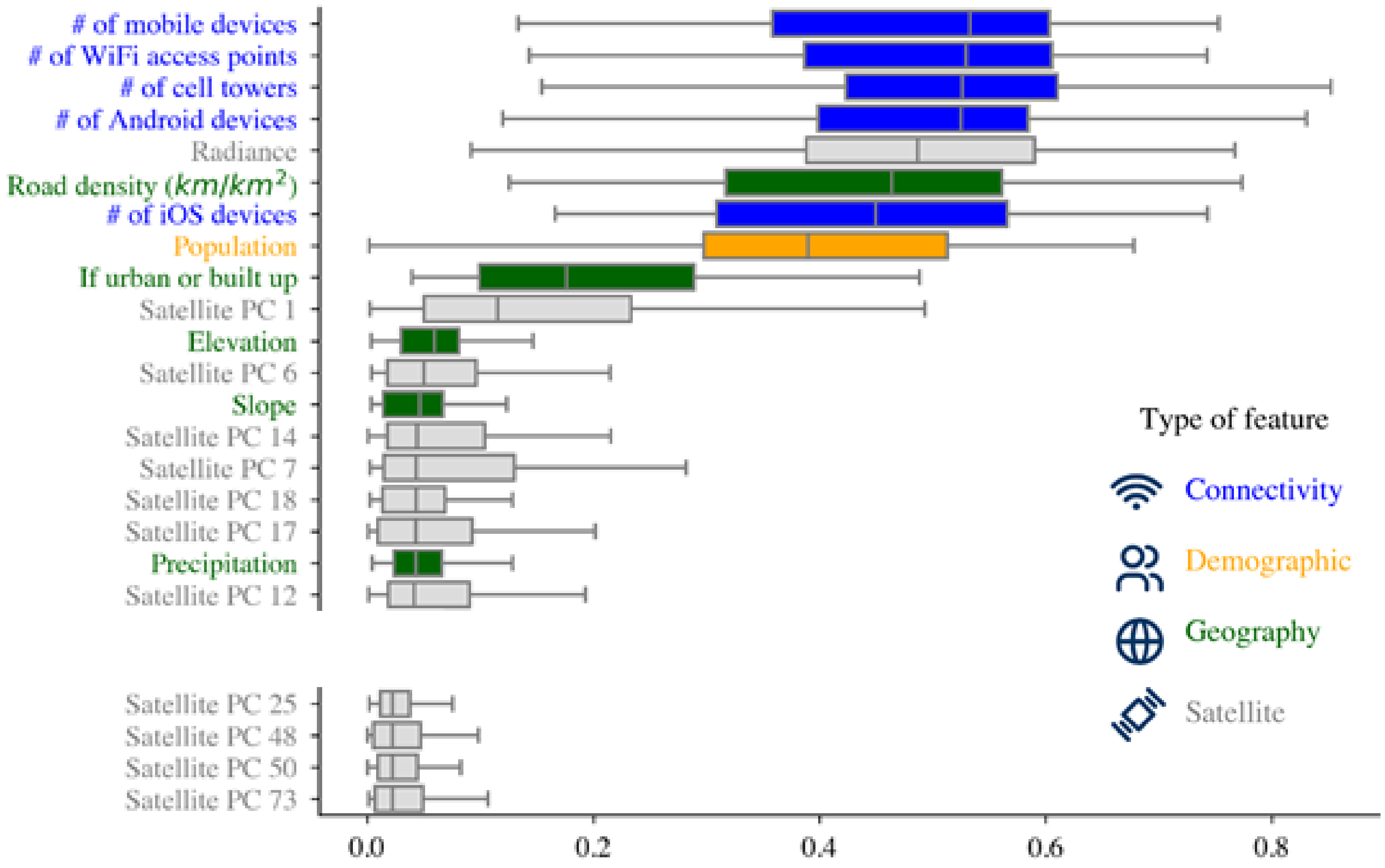
Feature Importance

- Intuitively, the features that “matter”:
  - Occur high in the tree (high information gain for that tree)
  - Occur frequently in the tree (if feature is non-binary)
  - Occur in many trees (if it’s a forest)

Feature Importance: Example



Feature Importance: Example



Feature Importance

- Formally, two common approaches:
  1. **Mean decrease impurity (aka Gini importance)**: average (across trees) decrease in weighted impurity caused by that feature

```python
from sklearn.datasets import load_boston
from sklearn.ensemble import RandomForestRegressor
import numpy as np
#Load boston housing dataset as an example
boston = load_boston()
X = boston["data"]
Y = boston["target"]
names = boston["feature_names"]
rf = RandomForestRegressor()
rf.fit(X, Y)
print "Features sorted by their score:"
print sorted(zip(map(lambda x: round(x, 4), rf.feature_importances_), names),
             reverse=True)
```

```
Features sorted by their score:
[(0.5298, 'LSTAT'), (0.4116, 'RM'), (0.0252, 'DIS'), (0.0172, 'CRIM'), (0.0065, 'NOX'),
(0.0035, 'PTRATIO'), (0.0021, 'TAX'), (0.0017, 'AGE'), (0.0012, 'B'), (0.0008, 'INDUS'),
(0.0004, 'RAD'), (0.0001, 'CHAS'), (0.0, 'ZN')]
```

Feature Importance

- Issues with impurity:
  - Biased towards features with multiple values
  - What happens when two features are closely correlated?

```
size = 10000
np.random.seed(seed=10)
X_seed = np.random.normal(0, 1, size)
X0 = X_seed + np.random.normal(0, .1, size)
X1 = X_seed + np.random.normal(0, .1, size)
X2 = X_seed + np.random.normal(0, .1, size)
X = np.array([X0, X1, X2]).T
Y = X0 + X1 + X2

rf = RandomForestRegressor(n_estimators=20, max_features=2)
rf.fit(X, Y);
print "Scores for X0, X1, X2:", map(lambda x:round (x,3),
                                    rf.feature_importances_)
```

```
Scores for X0, X1, X2: [0.278, 0.66, 0.062]
```

Feature Importance

- Formally, two common approaches:
  1. **Mean decrease impurity**: average (across trees) decrease in weighted impurity caused by that feature
  2. **Mean decrease accuracy ("Permutation Importance")**: average (across trees) decrease in performance when a given feature is randomized
     - Not implemented in sklearn (but very easy to do so by hand - see ESLII reading)

Feature Importance

- Issues
  - Interpret feature importances at your own risk!
  - They are informative, but rather atheoretical

Recap

- Regression
  - Parametric, fast training, linear
- Nearest Neighbors
  - Non-parametric, no training, complex decisions
- Naïve Bayes
  - Parametric, very fast training
- Decision Trees
  - Non-linear decisions, intuitive model

Key Concepts (this lecture)

- Regression vs. Decision trees
- Recursive regression trees algorithm
- Random forests
- Bagging
- Stacking
- Adaboost
- Gradient boosting
- Feature importance

For Next Class:

- Read:
  - Daume, chapters 4 and 10

- Keep working on Problem Set 4!