Machine Learning for Networks: Trees and ensembles

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ML methods

	ML task	Linear Regression	Logistic Regression	Tree-based learning	Neural Networks	k-Neirest Neighbors
Supervised	Regression	x			x	
	Classification		x	x	x	
Unsupervised	Clustering				x	x
	Dimensionality reduction				x	
	Anomaly detection			x	x	x
	Recommender Systems				x	

Outline

Decision tree

- Training: CART algorithm
- Entropy, Gini inpurity, Information Gain
- High variance

Ensemble learning

- Bagging
- Random Forest
- Extra trees

Interpretability

Case Study: Activity Classification

Problem:

- Authorities want to predict impact of a new infrastructure or service is introduced- ex. autonomous vehicles
- ... before making the investment
- We need *models* to predict user's behavior
- Traditional surveys are costly and have low penetration

Idea:

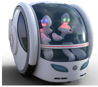
- Automatically sense user behavior via a smartphone app (Future Mobility Sensing - FMS)

In [KPZ+14]:

- Data collected via FMS
- Goal: classify each activity in *Home* or *Work*.
- Sample = Activity
- Features:

Age of the individual, time of day, duration, phone use, girometer data, accelerometer, GPS, etc.

Massachusetts Institute of Technology

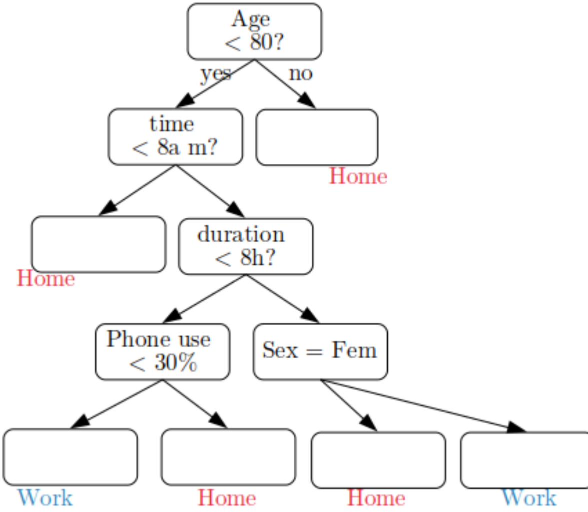


Section 1

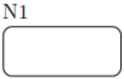
Decision tree

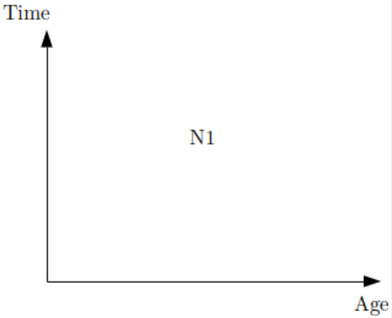
Decision Tree: Introduction

- Set of *splitting rules* organized as a tree.
- A class associated to each terminal node.
- Each sample traverses the tree up to a terminal node.
- Where does the following sample fall?
  age 50, time 10am, duration 7h, phone use 2%, sex Male

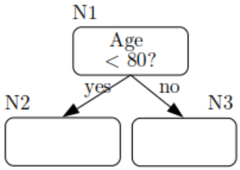


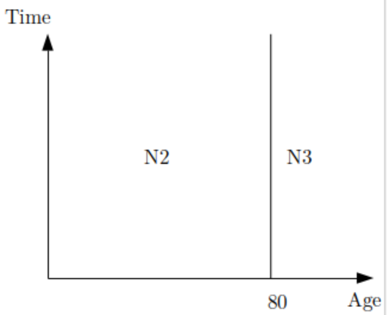
Nodes and regions



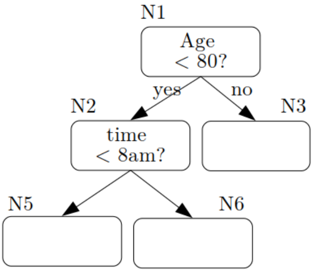


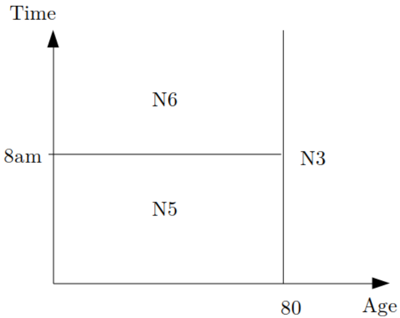
Nodes and regions





Nodes and regions





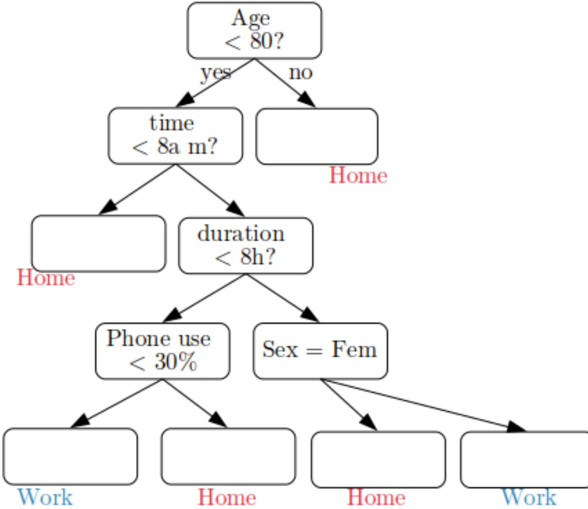
Question: Are random trees linear classifiers?

aa: No, the decision boundary is not linear

Training a decision tree

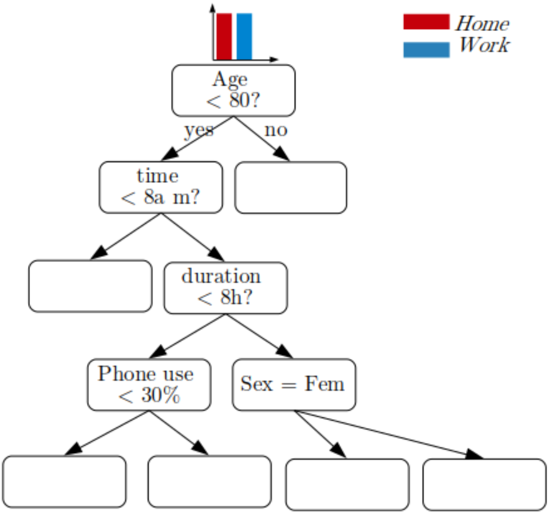
Decide:

- The label of each node
- the splitting rules at each node



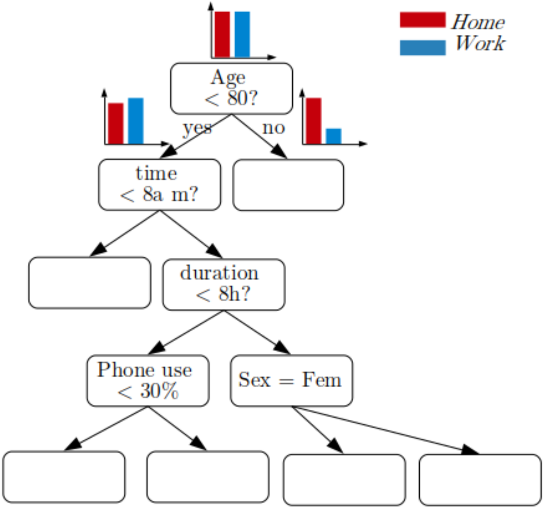
Assign labels to nodes

- How do we assign classes to the nodes?
  - Feed the tree with all the training samples



Assign labels to nodes

- How do we assign classes to the nodes?
  - Feed the tree with all the training samples
  - Observe the samples falling in each node and compute the histogram



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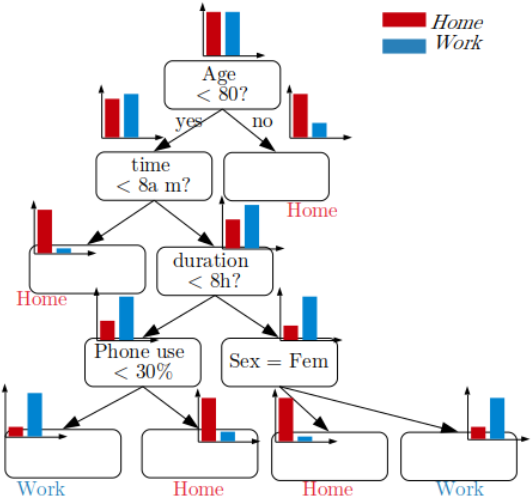
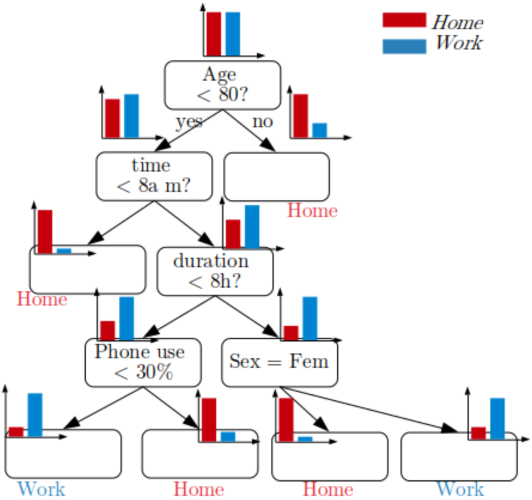


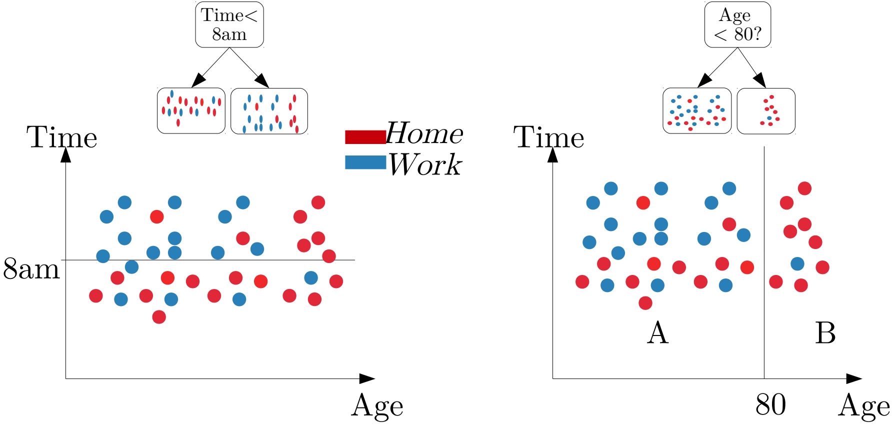
Assign labels to nodes

- How do we assign classes to the nodes?
  - Feed the tree with all the training samples
  - Observe the samples falling in each node and compute the histogram
  - Associate a node to its *prevalent class*.



Decide splitting rules

- We want a tree with just two terminal nodes. How do we choose the splitting rule?
- Which splitting rule is better?



Two metrics for impurity: *entropy* or *Gini impurity* index.

Entropy of a set of samples

Given a set of samples S

- p_b, p_r: ratio of samples in S that are blue / red.
- The entropy of S is defined as:

$$H(S) \triangleq p_b \cdot \log_2 \frac{1}{p_b} + p_r \cdot \log_2 \frac{1}{p_r}$$

Compute $H(A), H(B)$

Other examples:
$H(D) = 0.17 \cdot \log_2(1/0.17) + 0.83 \log_2(1/0.83) = 0.92$
$H(E) = 0.17 \cdot \log_2(1/0.17) + 0.83 \log_2(1/0.83) = 0.65$

The entropy measures the uncertainty about the class of each sample.
We can extend it to > 2 classes.

Information Gain

- Average entropy of the subsets

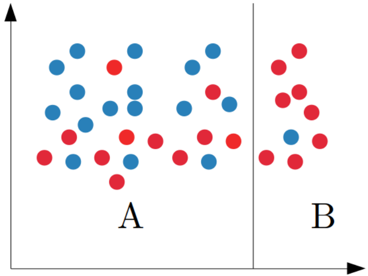
$$H(A,B) \triangleq p_A \cdot H(A) + p_B \cdot H(B)$$

where p_A, p_B are the ratios of samples in A and B.

- **Theorem**: partitioning a set always decreases the entropy (i.e. uncertainty):

$$H(A \cup B) \geq H(A,B)$$

- Knowing whether a sample is in A or B gives us additional info about its class.

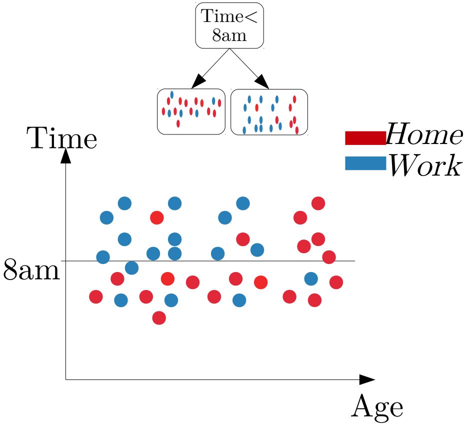


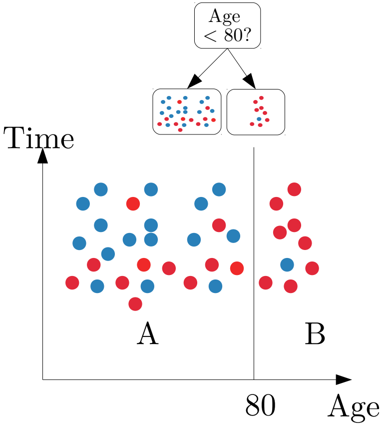
Information gain of a split:
$G \triangleq H(A \cup B) - H(A,B)$

$$\implies G \geq 0$$

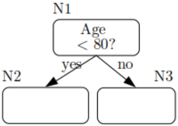
Information Gain of a Splitting Rule

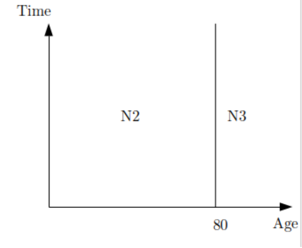
- A splitting rule partitions the samples
- We can associate a G to each splitting rule: G(Age<80), G(Time<8am)
- We prefer the rule that ?......?





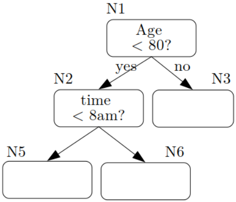
Information Gain of further Splitting Rules

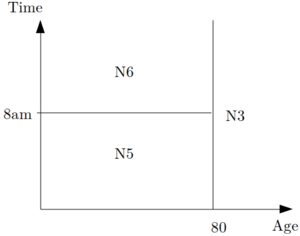




- We select Age<80 as our first splitting rule.
- After that, the information gain of Time<8am is

$$G = H(N2, N3) - H(\underbrace{N5, N6}_{\text{partition of N2}}, N3)$$



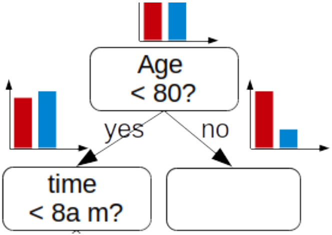


CART algorithm

We will *grow* (=train) our tree *on* our training set.

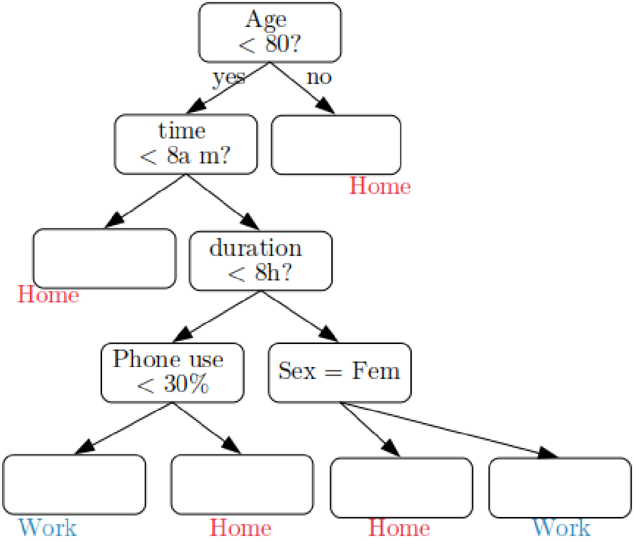
1. Decide the split points per each feature.
2. Compute a G per each
3. Select the (feature < split) with the highest G
4. Split the set of samples in two subsets (nodes)
5. Repeat the same process on each node

1. Age: 30, 40, 50, 60, 80
   Duration: 2,4,6,8 ...
2. G(Age<30)=0.3,
   G(Age<40)=0.32,
   ...,
   G(Duration<2)=0.4,
   G(Duration<4)=0.41, ...



CART = Classification and Regression Tree.

CART Algorithm: Result



Suboptimality of CART

- CART is a *greedy algorithm*:
  At every node it selects the "best" split, i.e., the one that maximizes the information gain
- Nothing ensures this is optimal: we may grow better trees by taking worse splits

Ex. If you want to make a lot of money.

- When you are 18, should you greedily work and get money?
- Or is it better to study first?

Other split metrics: Gini Impurity

- Entropy of a set S with K classes:

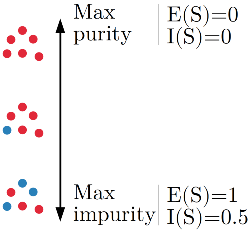
$$H(S) = \sum_{k=1}^{K} p_k \cdot \log_2 \frac{1}{p_k}$$

- Gini impurity of a set S:

$$I(S) = \sum_{k=1}^{K} p_k \cdot (1 - p_k)$$

  Probability that, taking any two samples from S, they are of the same class

- Conceptually similar to entropy.
- Impurity of a partition A, B:
  $I(A,B) = p_A \cdot I(A) + p_B \cdot I(B)$.
- Impurity of a split.



Other split metrics: Classification Error Rate

- Classification Error Rate of a set S: rate of error when classifying an element of S with its prevalent class

$$CER(S) = 1 - \max_k p_{k,S}$$

- CER of a partition A, B: $CER(A,B) = p_A \cdot CER(A) + p_B \cdot CER(B)$.
- CER of a split.
- Less used than entropy and Gini impurity.

Depth of a tree

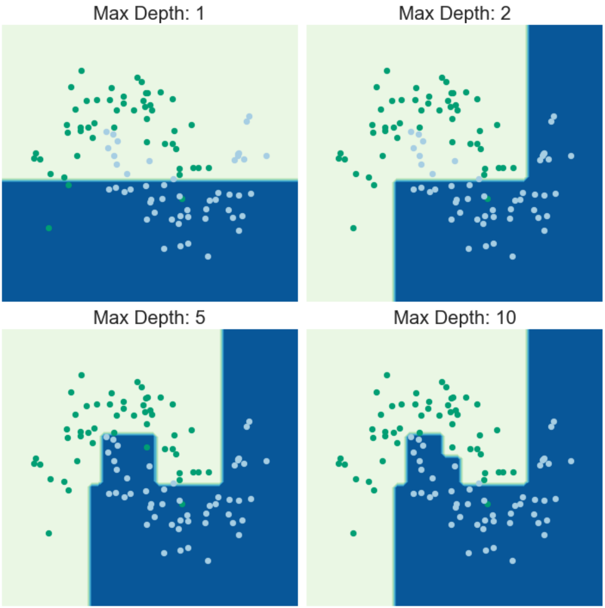
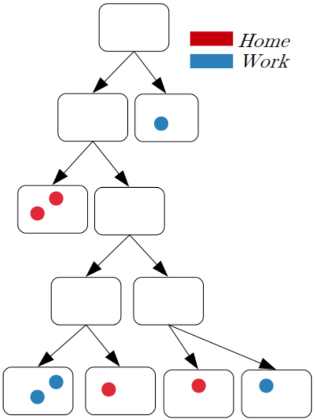


Image from *Pivotal, Pivotal Engineering Journal*:

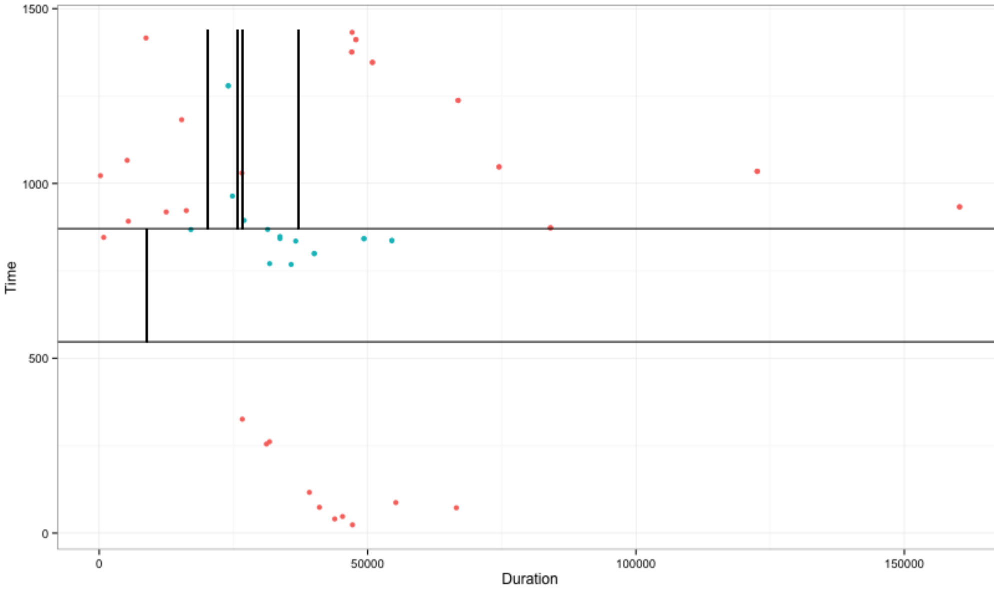
http://engineering.pivotal.io/post/interpreting-decision-trees-and-random-forests/

Depth of a tree

- CART stops when all terminal nodes are "pure"
- We say the tree is *fully grown*.



Overfitting



Prevent overfitting (regularization)

- *Pre-pruning*: We stop creating children at a node if
  - Too few samples at that node
  - Splitting does not give a high information gain.
  - The maximum number of nodes is reached
- *Post-pruning*: Develop a fully grown tree, then trim the nodes in a bottom-up manner
  - Use the validation data set to compute the Classification Error Rate.
  - Stop pruning if it reduces significantly.

These are all hyperparameters.

Section 2

Ensemble learning

The origin of variance in trees

From lesson 02.regression:

Variance

A model suffers **high variance** if, by perturbing a bit the training dataset, the model changes completely. Suppose $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ is a slightly perturbed version of $\mathbf{X}, \mathbf{y}$. If a model has high variance:

$$\begin{aligned} \tilde{\theta}^* &= \arg\min_\theta J(\theta, \tilde{\mathbf{X}}, \tilde{\mathbf{y}}) \\ \text{completely } \neq & \\ \theta^* &= \arg\min_\theta J(\theta, \mathbf{X}, \mathbf{y}) \end{aligned}$$

Example:
In our activity-classification use case, suppose you have training set $\mathbf{X}, \mathbf{y}$.

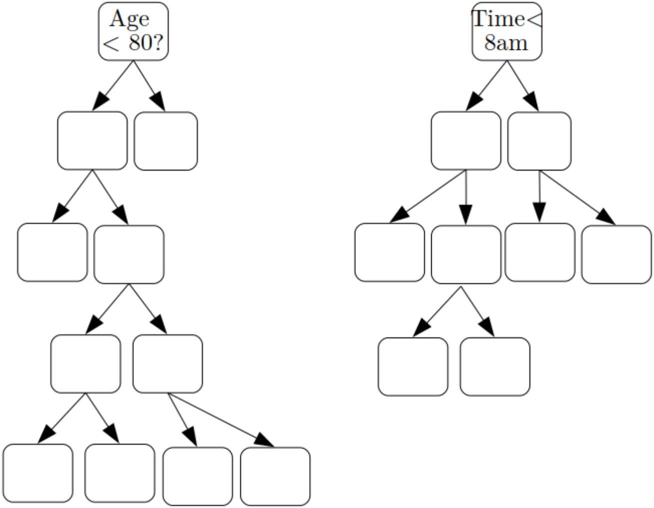
- CART decides the 1st splitting rule.
- Suppose $G(Age < 80) = 0.1002$ and $G(time < 8am) = 0.1000$.
- Which one does CART select?

If you had instead another training set $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ in which there is only another additional sample and
$G(Age < 80) = 0.1000$ and
$G(time < 8am) = 0.1001$.

- Which would be the 1st splitting rule selected by CART?

The origin of variance in trees

One sample only has changed completely our tree!



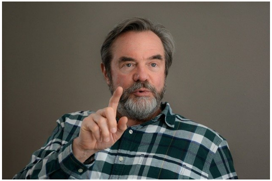
Would pruning solve this variance-problem?

aa: No, variance issue arises from the 1st splitting rule!

Ensembles

Why it works:

- If the President needs to face a pandemic, should he/she
  - Call the best expert in the world or
  - Call 10 good experts?
- A super-good expert can still make errors or be biased
- Plurality smooth errors and biases.



Ensemble methods

The following techniques have been proven empirically [BK11] to reduce the variance:

- Bagging
- Random Forests
- Extra Trees
- Boosting

Bagging

Training on a set $(\mathbf{X}, \mathbf{y})$

- *Boostrap sampling*:
  Obtain K subsets
  $(\mathbf{X}, \mathbf{y})_k \subseteq (\mathbf{X}, \mathbf{y})$
  - Set size can change
- Grow a tree $h_k(\cdot)$ on each $(\mathbf{X}, \mathbf{y})_k$

Prediction of a new $\mathbf{x}$

- Obtain $h_k(\mathbf{x})$ from each tree $h_k(\cdot)$
- Use *majority voting*

How many trees?

- Typically several hundreds.
- **Interpretability**: **feature importance**.

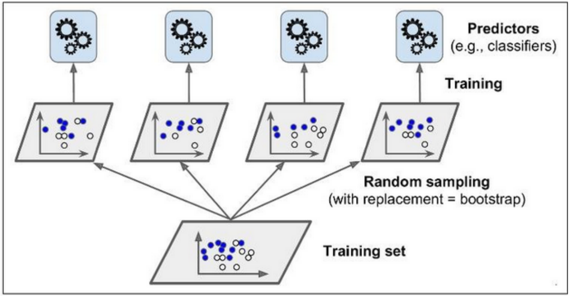


Figure 7-4. Bagging and pasting involves training several predictors on different random samples of the training set

From [Ger19]

Detail not important: If sampling is with replacement (the same sample can be taken multiple times when growing one tree), we talk about *bagging*. If instead sampling is without replacement, we talk about *Pasting*

Random forest

Modified version of bagging:

- Every time we decide the split rule, the candidate variables under considerations are a random subset.
- The inventors suggest $\sqrt{N}$ candidates ($N =$ num of features). However, it is a parameter to tune.

Advantages over Bagging

- **Less variance**, i.e., less overfitting
  - With bagging all trees tend to be the same at their top nodes $\Longrightarrow$ Trees are correlated.
  - Random forests create more de-correlated trees. $\Longrightarrow$ Predictions are more diverse.
  - (To face a pandemic, it is not worth having experts all thinking the same)
- Computation **efficiency**.

General lesson in ML: **stochasticity is your friend** to get (i) stable predictors, (ii) efficiency and (iii) interpretability.

Number of trees

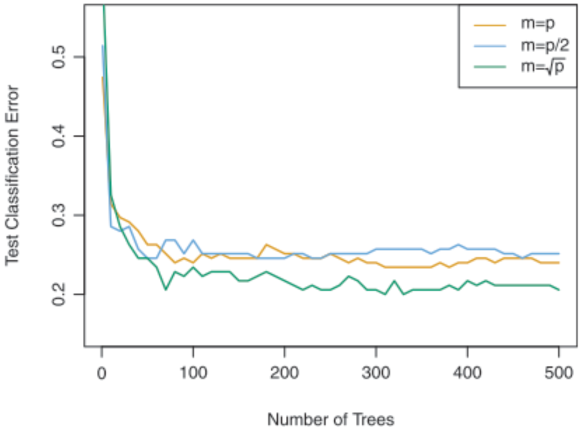
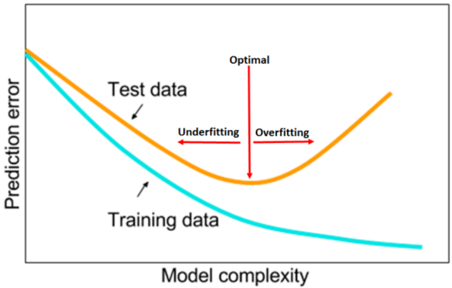


FIGURE 8.10. *Results from random forests for the 15-class gene expression data set with $p = 500$ predictors. The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree node. Random forests ($m < p$) lead to a slight improvement over bagging ($m = p$). A single classification tree has an error rate of 45.7%.*

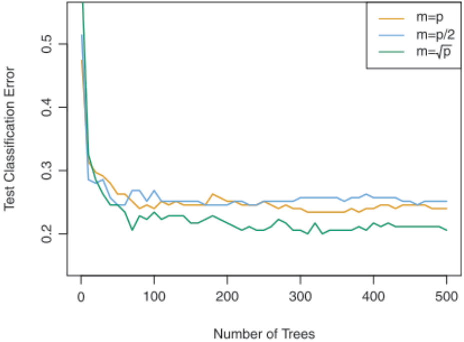
From [JWHT13]

No increase in complexity



From [Smi18]

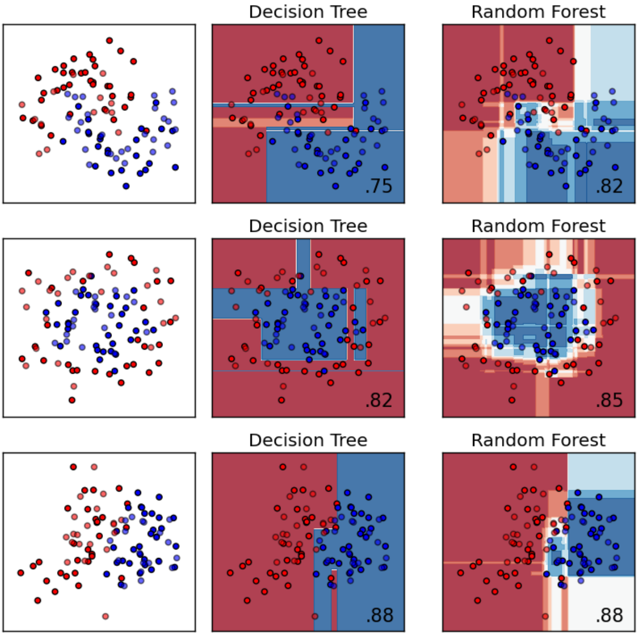
Adding neurons in a NN increases complexity



From [JWHT13]

Adding a predictor in an ensemble does not increase complexity
$\Longrightarrow$ We don't increase the risk of overfitting

Classification boundaries



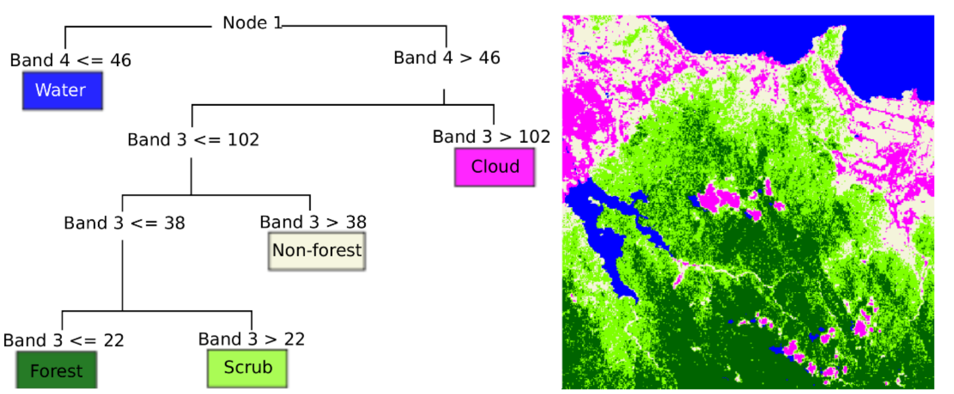
What does the shading represent?

Interpretability: Confidence in the prediction

Picture from Martin Thoma

Tree Classifier Application: Image Segmentation

- Predictors: red (band 3) and near-infrared (band 4) bands from the Landsat Enhanced Thematic Mapper Plus satellite sensor.



Ref: Horning N., *Random Forests : An algorithm for image classification and generation of continuous fields data sets*

Randomness in tree-based models

- Single Tree
- Bagging
  Sampling data points
- Random forests
  ++ Random features
- Extra-trees (extremely randomized trees)
  ++ Random splitting rule (instead of the best, as in CART)

Boosting

- Bagging, Random Forests and extra trees:
  - Each tree is independent
- Boosting:
  - Each tree tries to “correct” the errors of the others
  - Ex.: XGBoost

Applicable with Bagging Classification Trees, Random Forests and Extra-Forests.

Importance of a feature:[1]

- In each tree
  - Check all the rules which use that feature
  - Check the gain (either information gain or decrease in Gini impurity index)
  - Sum all these gains
- Score: Average the per-tree gain over all the trees (weighting with the samples-per-tree)

Scale all the feature scores so that they sum up to 1.

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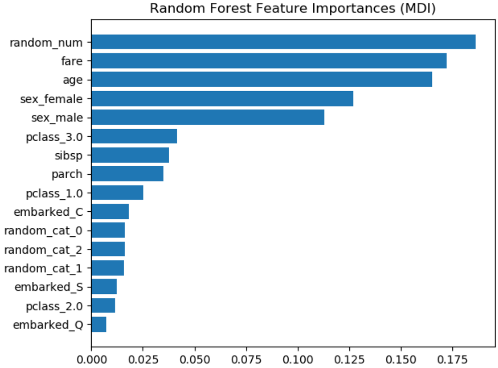
[1] See pagg.198-199 of [Ger19] and pagg.333-334 of [JWHT13]

Interpretability: Feature Importance



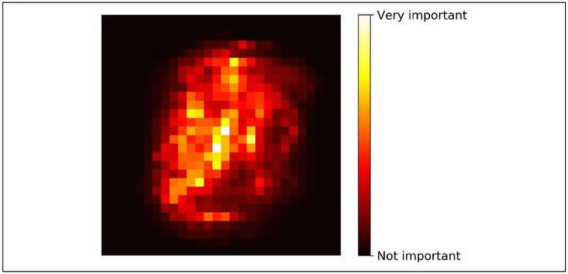


Figure 7-6. MNIST pixel importance (according to a Random Forest classifier)

From Scikit Learn docs
and from [Ger19]

Scaling needed?

aa: No, as every time we decide a splitting rule, the threshold is automatically chosen in the range of the feature considered.

Tree Regressor

- Predicted value = avg of samples of a tree node
- Training = Find splits that minimize the Mean Squared Error (MSE)

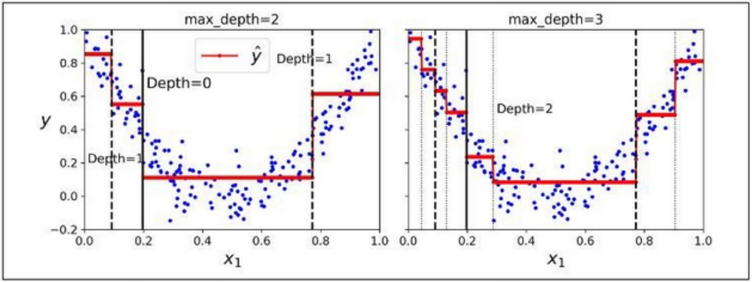


Figure 6-5. Predictions of two Decision Tree regression models

From [Ger19].

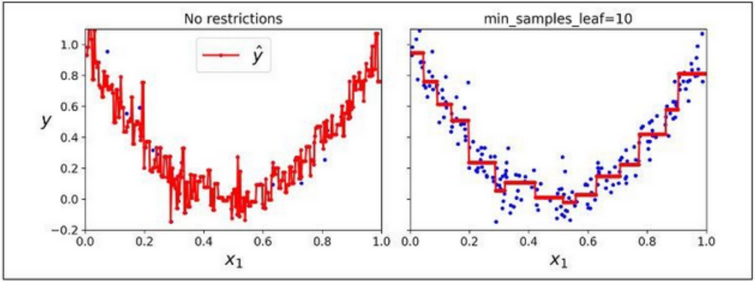


Figure 6-6. Regularizing a Decision Tree regressor

Decision tree

- Training: CART algorithm
- Entropy, Gini inpurity, Information Gain
- High variance

Ensemble learning

- Bagging
- Random Forest
- Extra trees

Interpretability

Suggested Reading

Ian H. Witten, Eibe Frank, Mark A. Hall. Data Mining: Practical Machine Learning Tools and Techniques 2nd Edition Elsevier - Section 6.1

References I

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- Youngsung Kim, Francisco C. Pereira, Fang Zhao, Ajinkya Ghorpade, P. Christopher Zegras, and Moshe Ben-Akiva, *Activity recognition for a smartphone based travel survey based on cross-user history data*, International Conference on Pattern Recognition (2014).
- Leslie N. Smith, *A disciplined approach to neural network hyper-parameters: Part 1 – learning rate, batch size, momentum, and weight decay*, Tech. report, US Naval Research Laboratory, 2018.