

Machine Learning for Networks: Trees and ensembles

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

Decision tree

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

Ensemble learning

- Bagging
- Random Forest
- Extra trees

Interpretability

Case Study: Activity Classification

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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



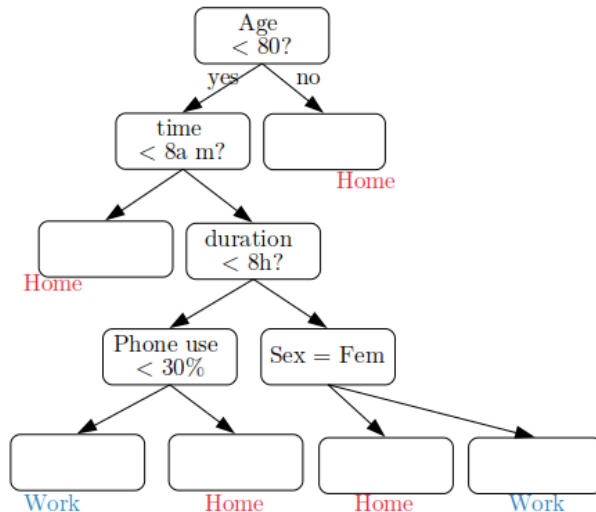
Section 1

Decision tree

Decision Tree: Introduction

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- 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

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N1



Time



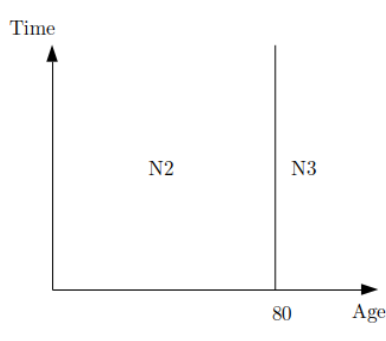
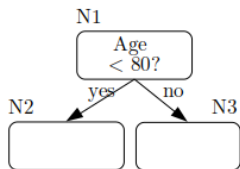
N1

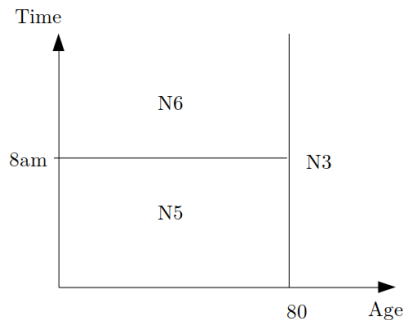
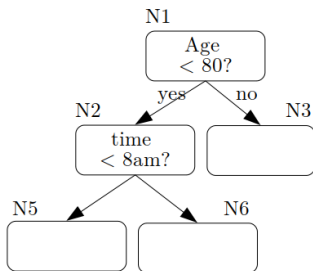
Age



Nodes and regions

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Question: Are random trees linear classifiers?

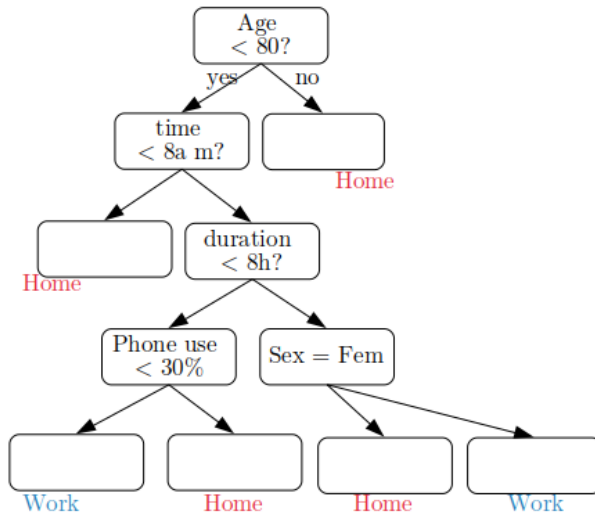
aa: No, the decision boundary is not linear

Training a decision tree

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Decide:

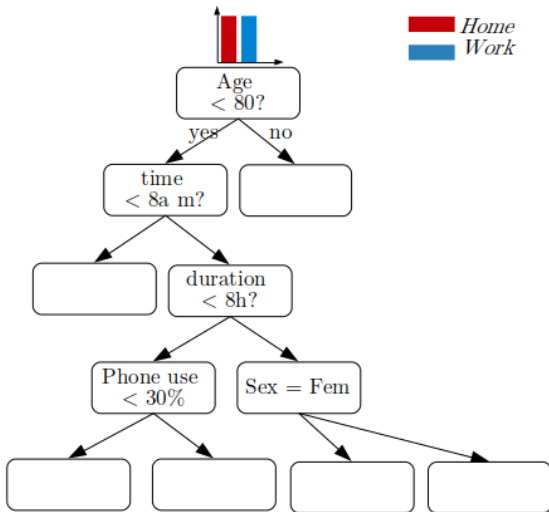
- The label of each node
- the splitting rules at each node



Assign labels to nodes

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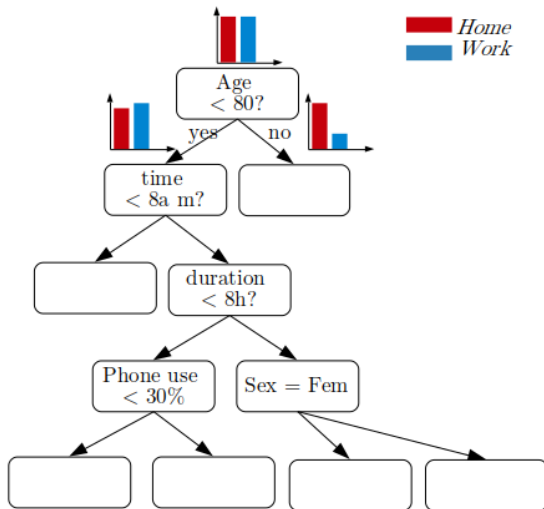
- How do we assign classes to the nodes?
 - Feed the tree with all the training samples



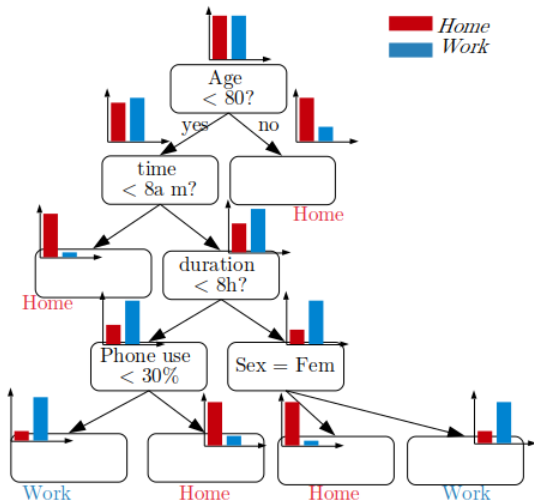
Assign labels to nodes

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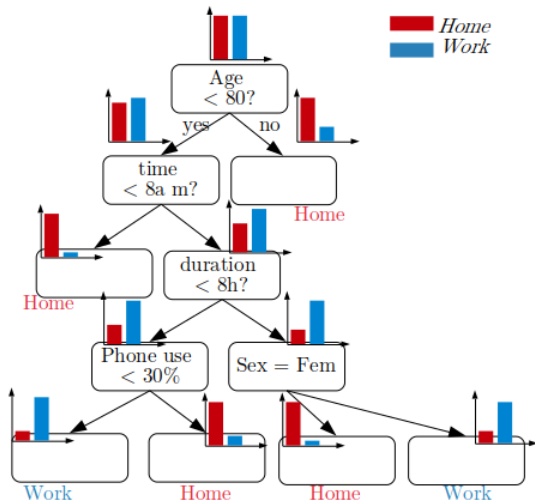
- How do we assign classes to the nodes?
 - Feed the tree with all the training samples
 - Observe the samples falling in each node and compute the histogram



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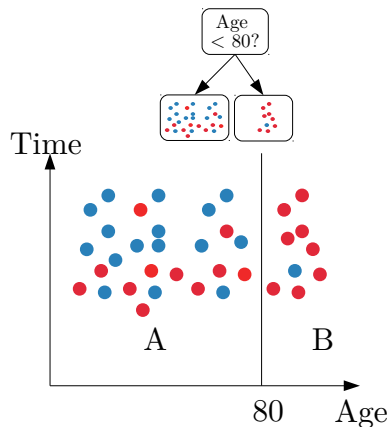
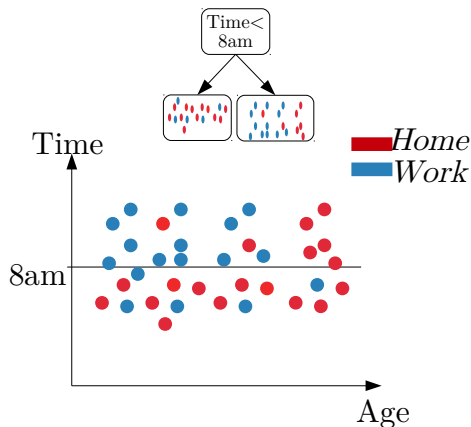
- How do we assign classes to the nodes?
 - Feed the tree with all the training samples
 - Observe the samples falling in each node and compute the histogram
 - Associate a node to its *prevalent class*.



Decide splitting rules

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- 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

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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.



- Average entropy of the subsets

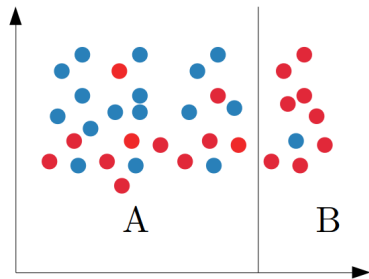
$$H(A,B) \triangleq p_A \cdot H(A) + p_B \cdot H(B)$$

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.



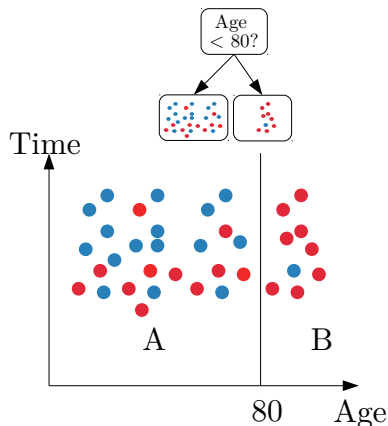
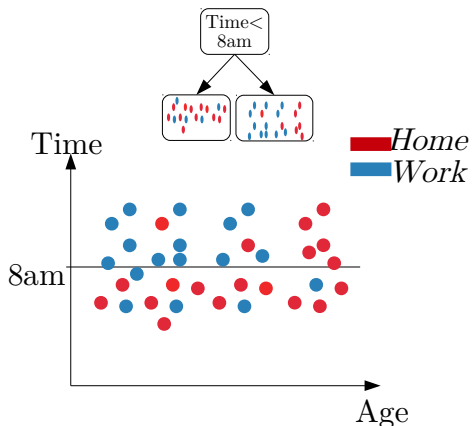
Information gain of a split:
 $G \triangleq H(A \cup B) - H(A,B)$

$$\implies G \geq 0$$

Information Gain of a Splitting Rule

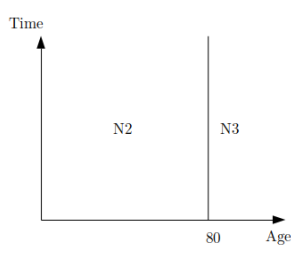
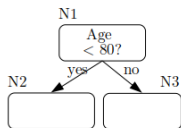
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- A splitting rule partitions the samples
- We can associate a G to each splitting rule: $G(\text{Age} < 80)$, $G(\text{Time} < 8\text{am})$
- We prefer the rule that ?.....?



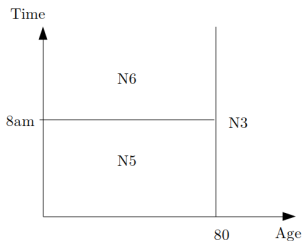
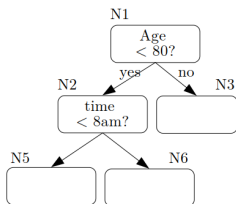
Information Gain of further Splitting Rules

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

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

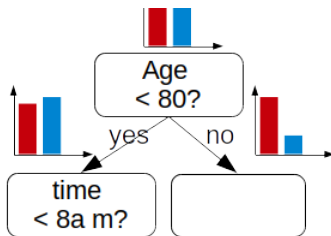


CART algorithm

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

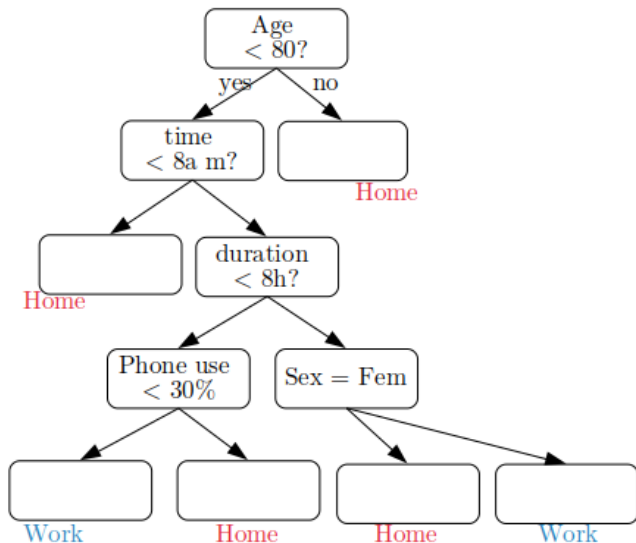
1. Decide the split points per each feature.
 2. Compute a G per each
 3. Select the (feature < split) with the highest G
 4. Split the set of samples in two subsets (nodes)
 5. Repeat the same process on each node
1. Age: 30, 40, 50, 60, 80
Duration: 2,4,6,8 ...
 2. $G(\text{Age} < 30) = 0.3$,
 $G(\text{Age} < 40) = 0.32$,
...,
 $G(\text{Duration} < 2) = 0.4$,
 $G(\text{Duration} < 4) = 0.41$, ...



CART = Classification and Regression Tree.

CART Algorithm: Result

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- 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?

- Entropy of a set S with K classes:

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

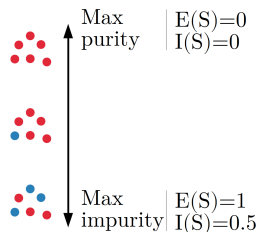
- Gini impurity of a set S :

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

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.

With two classes:



With more than 2 classes,
we may have $E(S) > 1$ and
 $I(S) > 1$

- 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.

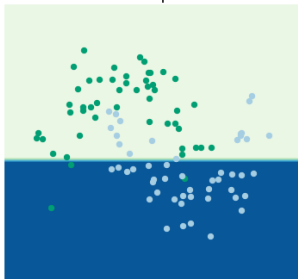
Depth of a tree

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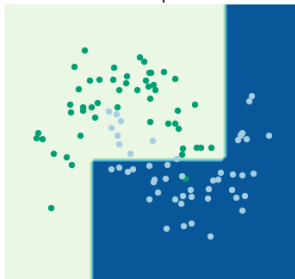
Image from *Pivotal, Pivotal Engineering Journal*:

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

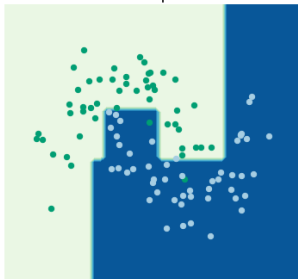
Max Depth: 1



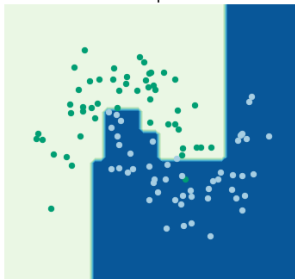
Max Depth: 2



Max Depth: 5



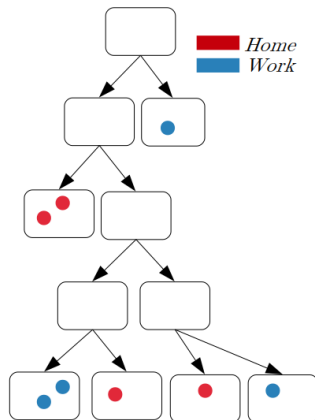
Max Depth: 10



Depth of a tree

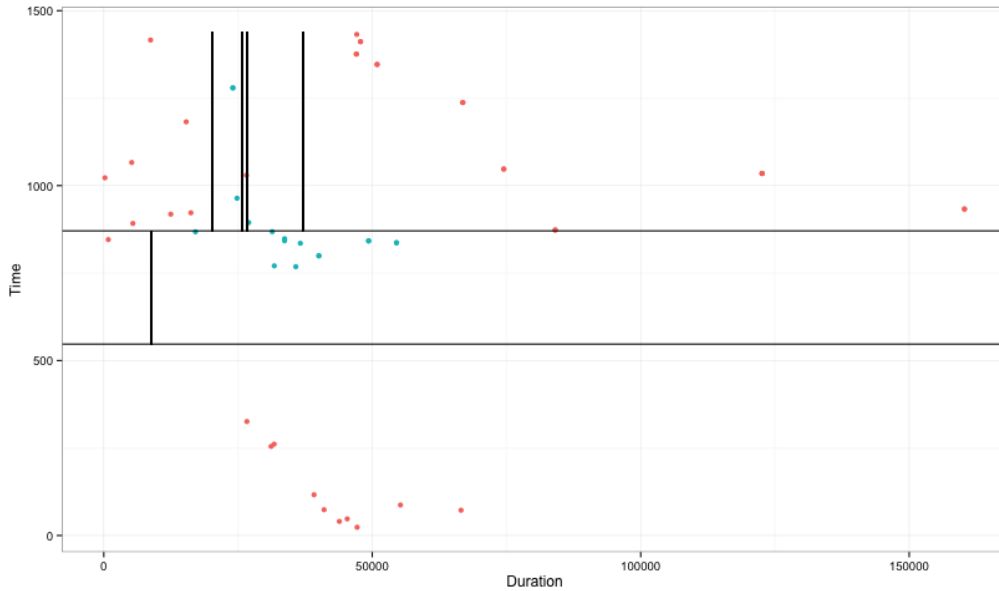
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- CART stops when all terminal nodes are “pure”
- We say the tree is *fully grown*.



Overfitting

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- *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

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:

$$\tilde{\theta}^* = \arg \min_{\theta} J(\theta, \tilde{\mathbf{X}}, \tilde{\mathbf{y}})$$

completely \neq

$$\theta^* = \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

Example:

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

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

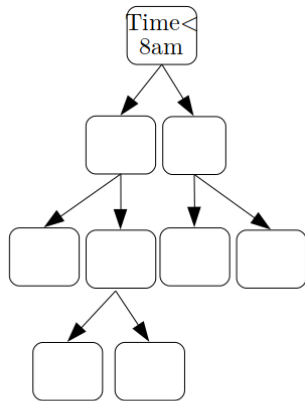
If you had instead another training set $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ in which there is only another additional sample and

$G(\text{Age} < 80) = 0.1000$ and
 $G(\text{time} < 8am) = 0.1001$.

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

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```
graph TD; A[Age < 80?] --> B[ ]; A --> C[ ]; B --> D[ ]; B --> E[ ]; C --> F[ ]; F --> G[ ]; F --> H[ ]; E --> I[ ]; E --> J[ ]
```



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

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.



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

- Bagging
- Random Forests
- Extra Trees
- Boosting

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

- *Bootstrap 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.**

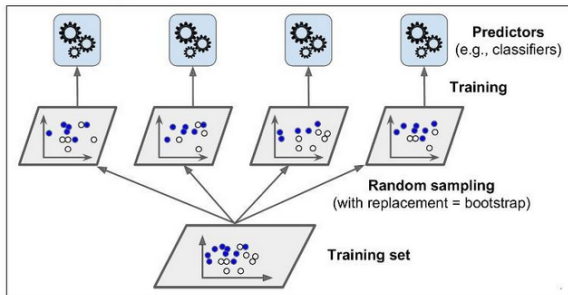


Figure 7-4. Bagging and pasting involves training several predictors on different random samples of the training set

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*

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 ($N = \text{num of features}$).
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
 \implies Trees are correlated.
 - Random forests create more de-correlated trees.
 \implies 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.

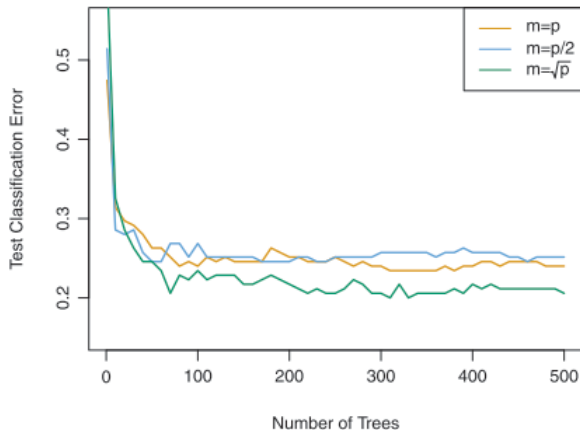
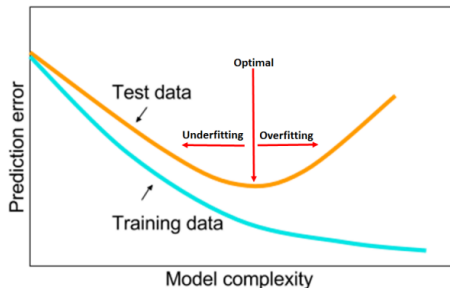


FIGURE 8.10. Results from random forests for the 15-class gene expression data set with $p = 500$ predictors. The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m , the number of predictors available for splitting at each interior tree 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%.

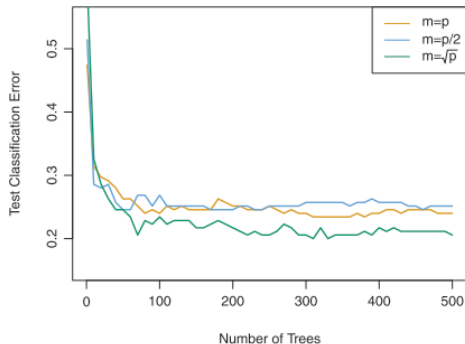
No increase in complexity

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From [Smi18]

Adding neurons in a NN increases complexity



From [JWHT13]

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

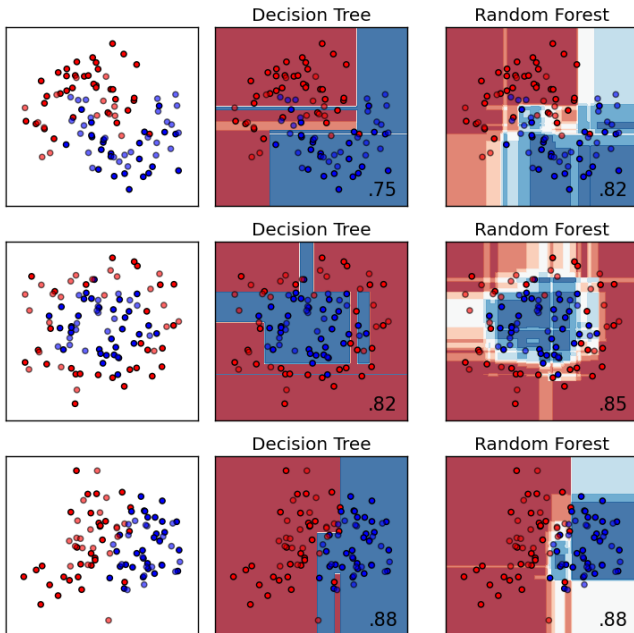
Classification boundaries

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What does the shading represent?

**Interpretability:
Confidence in the
prediction**

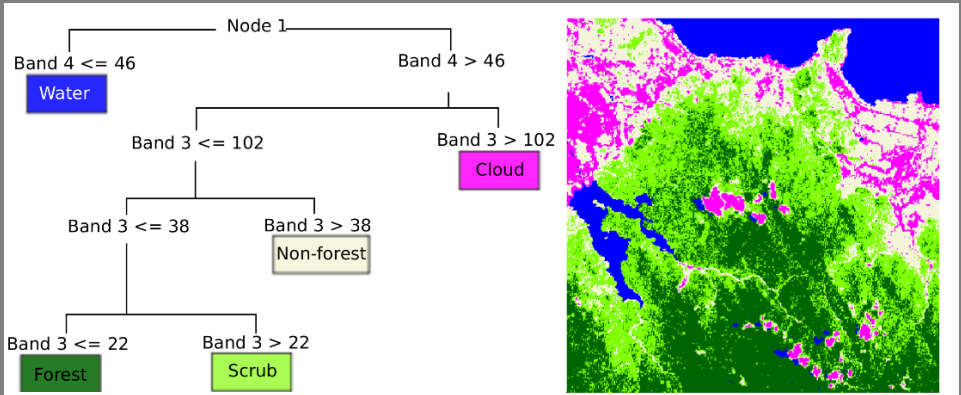
Picture from [Martin Thoma](#)



Tree Classifier Application: Image Segmentation

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- 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*

- 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)

- 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

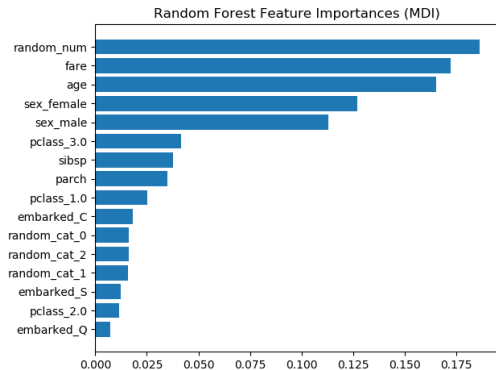
- In each tree
 - Check all the rules which use that feature
 - Check the gain (either information gain or decrease in Gini impurity index)
 - Sum all these gains
- Score: Average the per-tree gain over all the trees (weighting with the samples-per-tree)

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

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

Interpretability: Feature Importance

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From [Scikit Learn docs](#)
and from [\[Ger19\]](#)

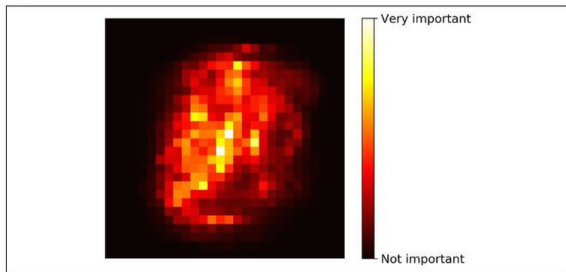


Figure 7-6. MNIST pixel importance (according to a Random Forest classifier)

Scaling needed?

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

Tree Regressor

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

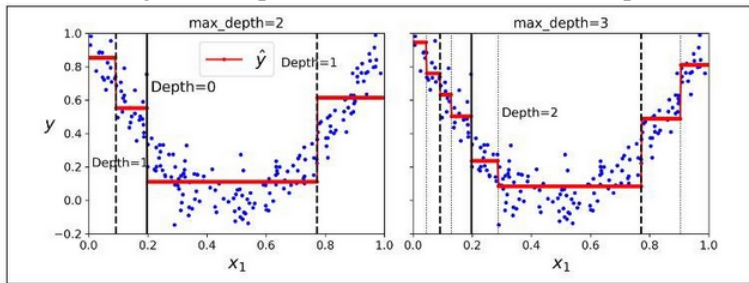


Figure 6-5. Predictions of two Decision Tree regression models

From [Ger19].

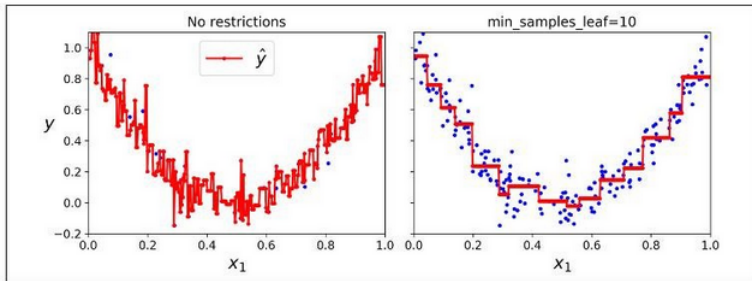


Figure 6-6. Regularizing a Decision Tree regressor

Decision tree






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

Ensemble learning

- Bagging
- Random Forest
- Extra trees

Interpretability

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

-  Eric Bauer and Ron Kohavi, *An Empirical Comparison of Voting Classification Algorithms : Bagging , Boosting , and Variants*, Machine Learning **38** (2011), no. 1998, 1–38.
-  Aurelien Geron, *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, O'Reilly, 2019.
-  Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani, *An introduction to Statistical Learning*, vol. 7, 2013.
-  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.