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	

Decision tree

- Training: CART algorithm
- Entropy, Gini inpurity, Information Gain
- Instability

Ensemble learning

- Bagging
- Random Forest
- Extra trees

Interpretability

Famous example

Microsoft Kinect (Xbox)[KS13]

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:

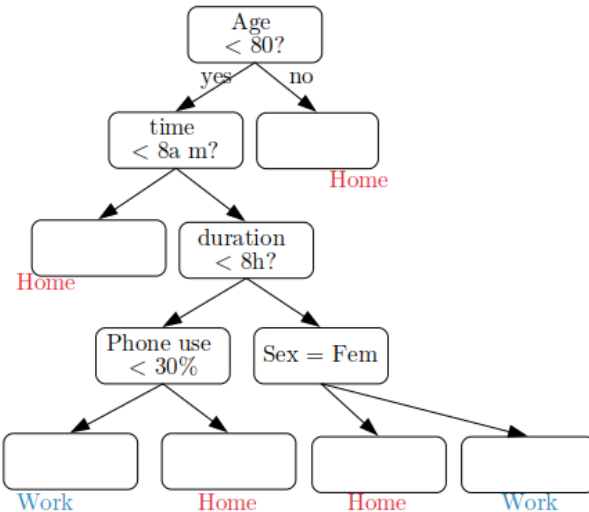
Age of the individual, time of day, duration, phone use, girometer data, accelerometer, GPS, etc.

Section 1

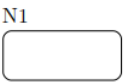
Decision tree

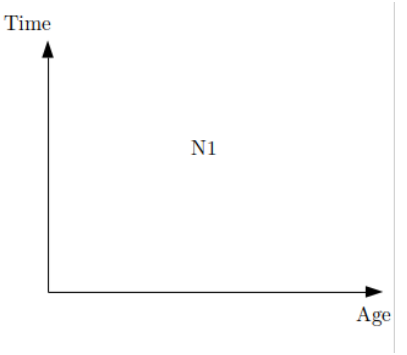
Decision Tree: Introduction

- 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





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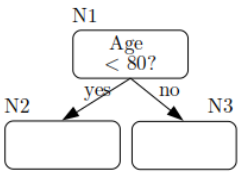

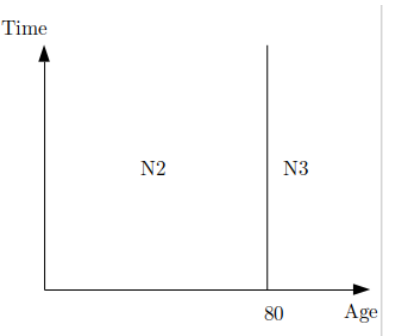

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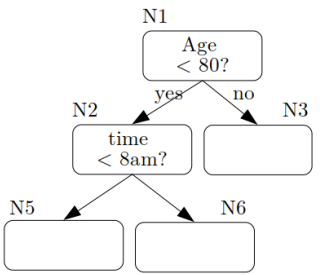
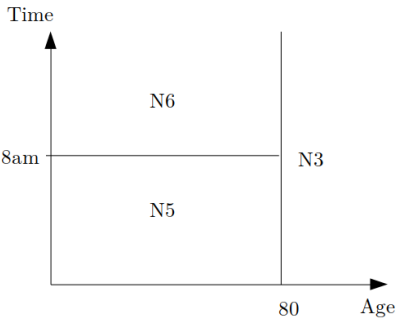


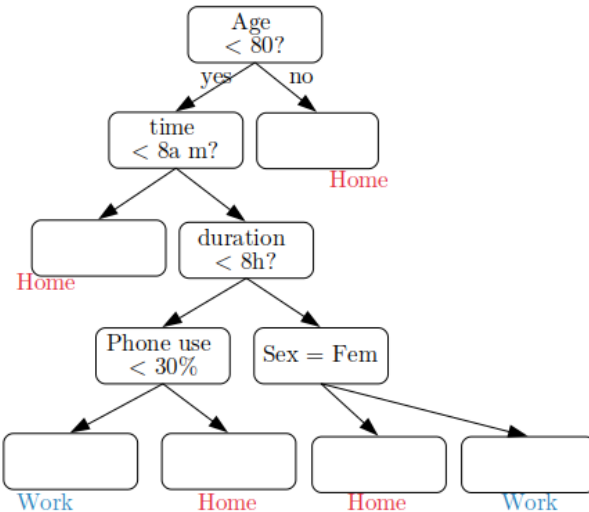


Question: Are decision trees linear classifiers?

Training a decision tree

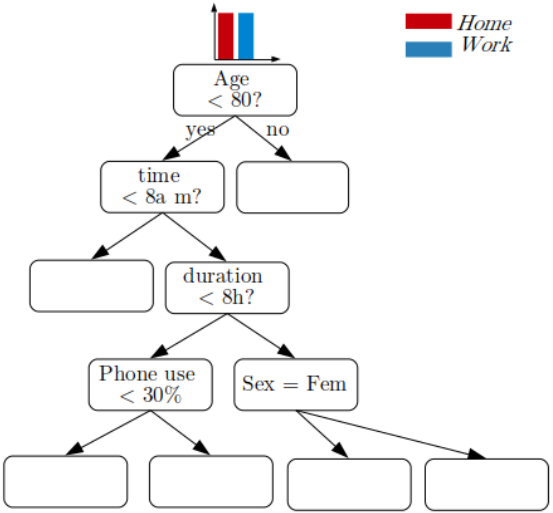
Decide:

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



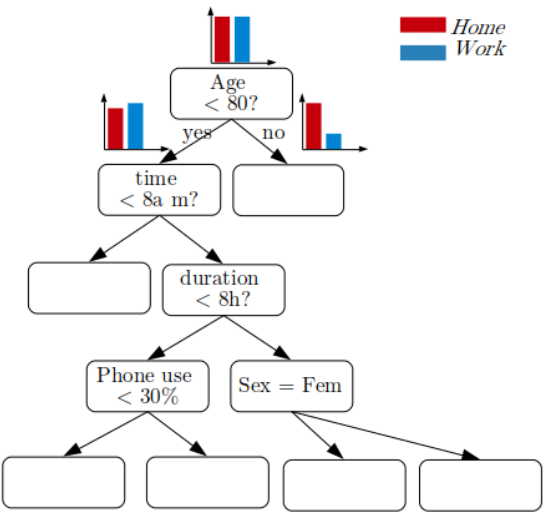
Assign labels to nodes

- 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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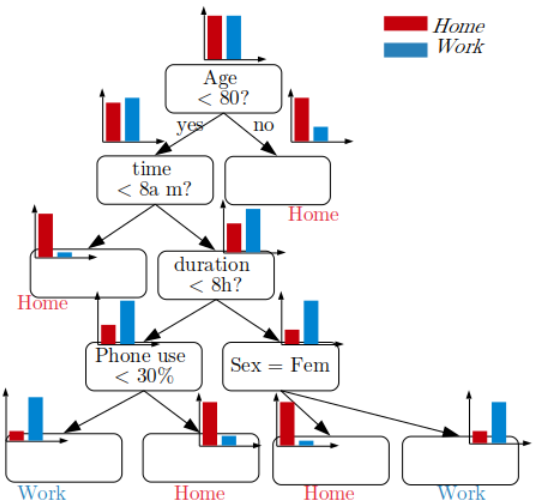
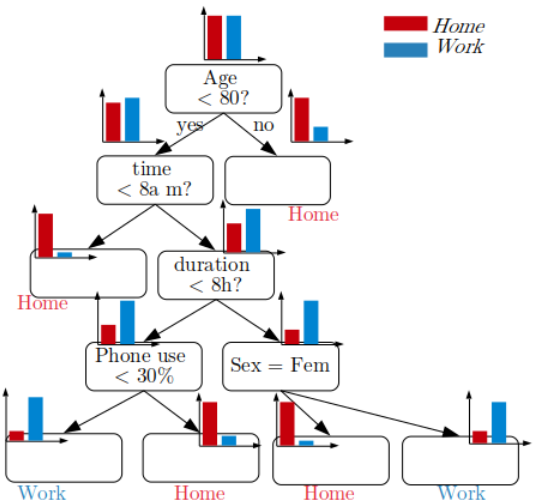


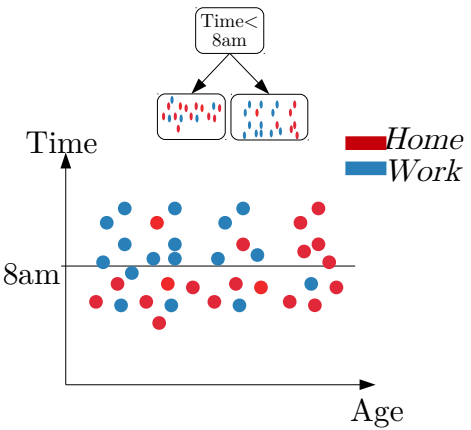
Assign labels to nodes

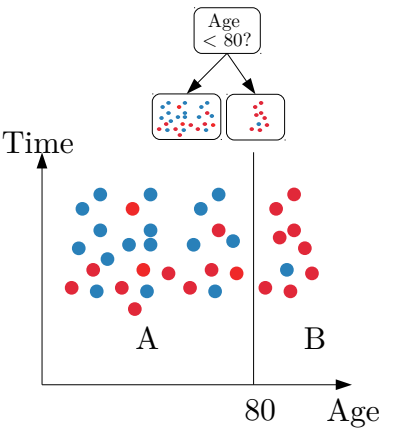
- How do we assign classes to the nodes?
  - Feed the tree with all the training samples
  - Observe the samples falling in each node and compute the histogram
  - Associate a node to its *prevalent class*.



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:
$H(D) = 0.33 \cdot \log_2(1/0.33) + 0.67 \log_2(1/0.67) = 0.91$
$H(E) = 0.17 \cdot \log_2(1/0.17) + 0.83 \log_2(1/0.83) = 0.65$

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

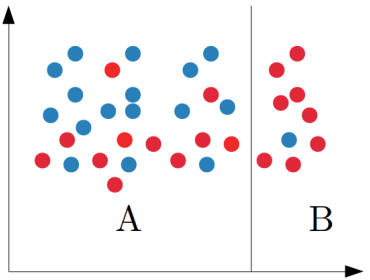
$$H(A,B) \triangleq p_A \cdot H(A) + p_B \cdot H(B)$$

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.

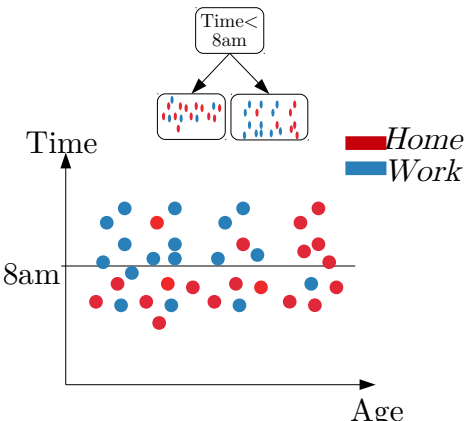


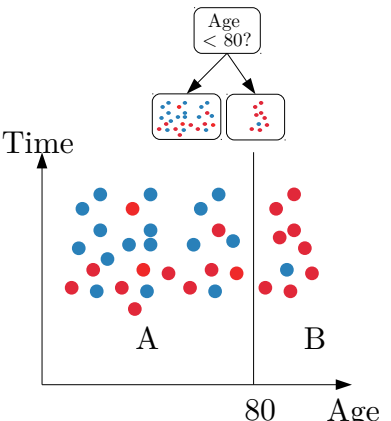
Information gain of a split:
$G \triangleq H(A \cup B) - H(A,B)$

$$\Longrightarrow G \geq 0$$

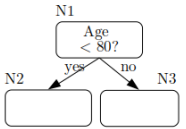
Information Gain of a Splitting Rule

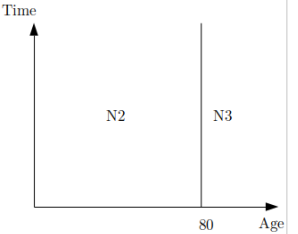
- A splitting rule partitions the samples
- We can associate a G to each splitting rule: G(Age<80), G(Time<8am)
- We prefer the rule that ?.....?





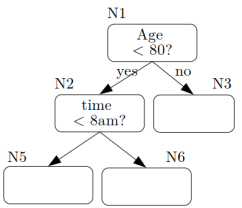
Information Gain of further Splitting Rules

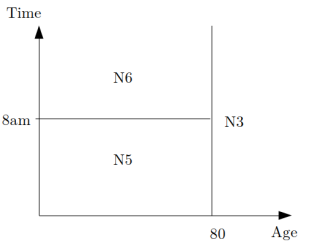




- We select Age<80 as our first splitting rule.
- After that, the information gain of Time<8am is

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



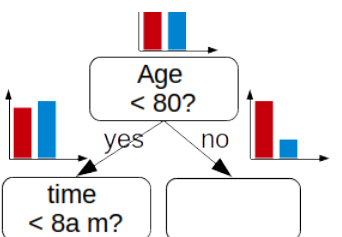


CART algorithm

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

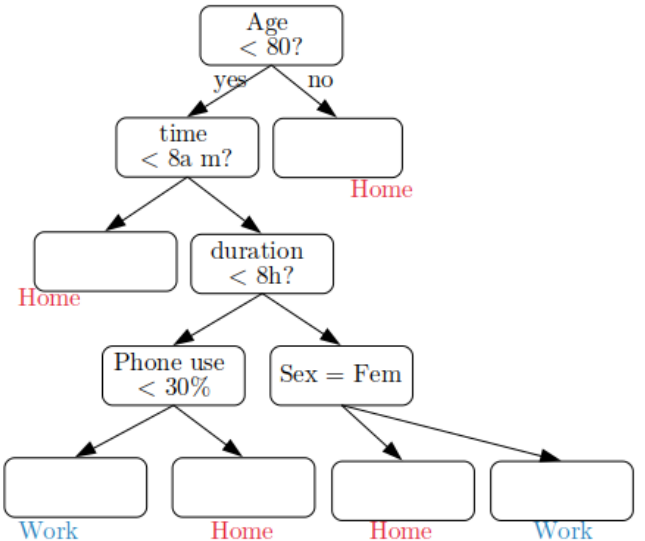
1. Decide the split points per each feature.
2. Compute a G per each
3. Select the (feature < split) with the highest G
4. Split the set of samples in two subsets (nodes)
5. Repeat the same process on each node

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:

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

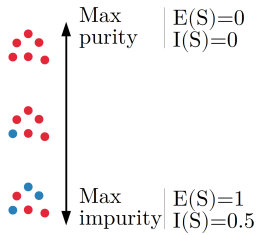
- Gini impurity of a set S:

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

  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.

With two classes:



In general

$0 \leq E(S) \leq \log_2 K$ and

$0 \leq I(S) \leq \frac{1}{K}$.

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

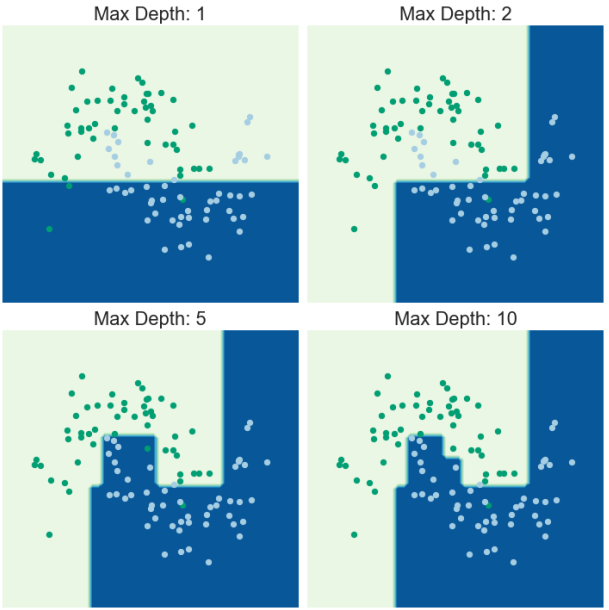
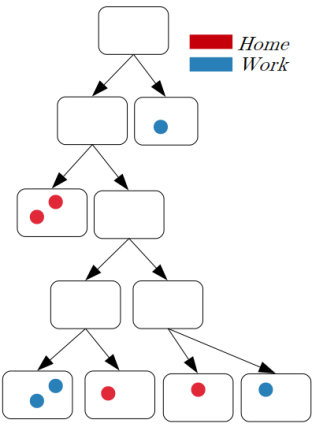


Image from *Pivotal, Pivotal Engineering Journal*:

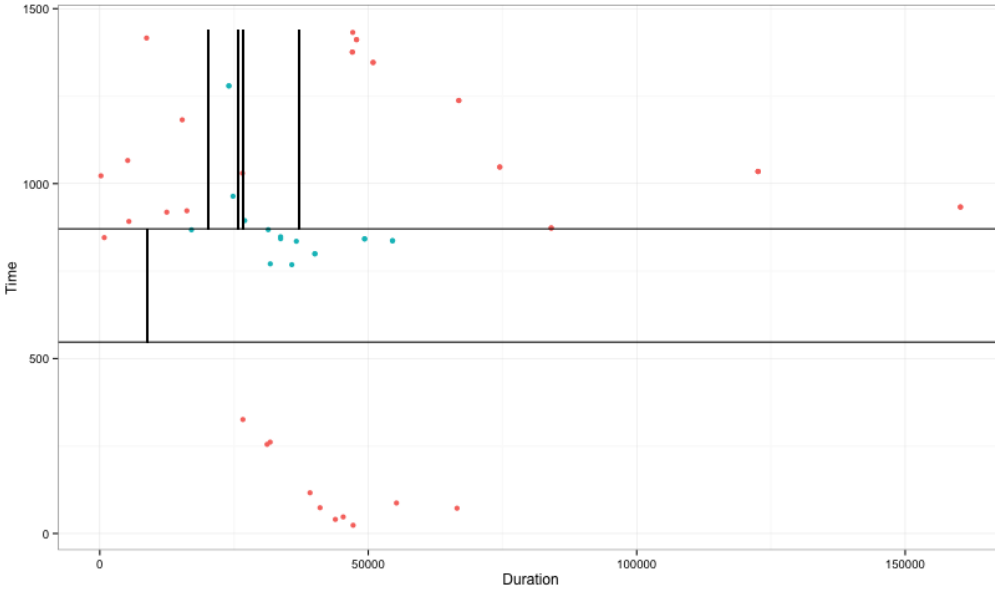
http://engineering.pivotal.io/post/interpreting-decision-trees-and-random-forests/

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 instability in trees

From lesson 02.regression:

Instability

A model is **unstable** 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 is unstable:

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

completely $\neq$

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

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

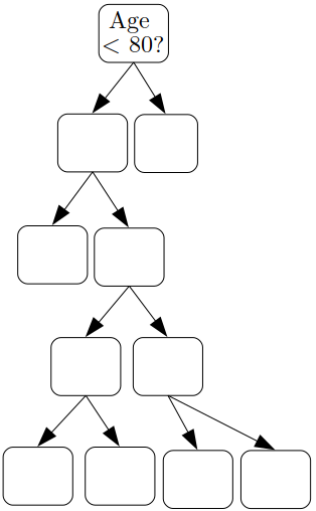
- CART decides the 1st splitting rule.
- Suppose $G(Age < 80) = 0.1002$ and $G(time < 8am) = 0.1000$.
- Which one does CART select?

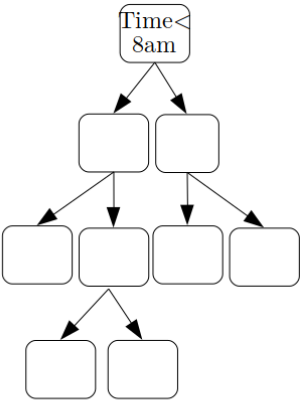
If you had instead another training set $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ in which there is only another additional sample and $G(Age < 80) = 0.1000$ and $G(time < 8am) = 0.1001$.

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

The origin of instability in trees

One sample only has changed completely our tree!





Would pruning solve this instability problem?

aa: No, instability 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.

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

- 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**.

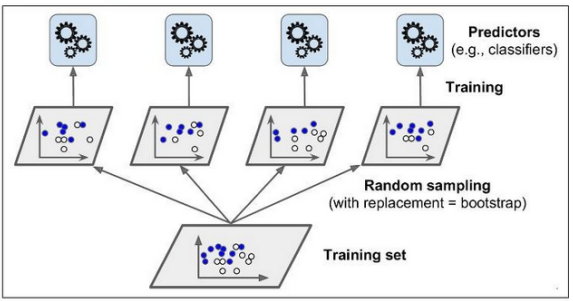


Figure 7-4. Bagging and pasting involves training several predictors on different random samples of the training set

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 instability**, 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

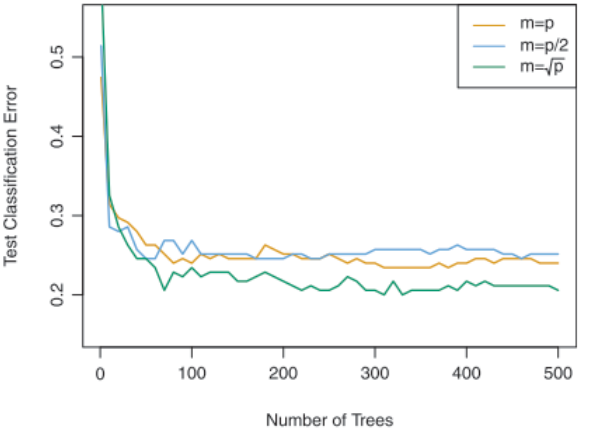
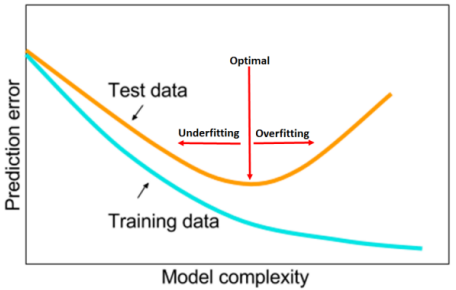


FIGURE 8.10. *Results from random forests for the 15-class gene expression data set with $p = 500$ predictors. The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree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

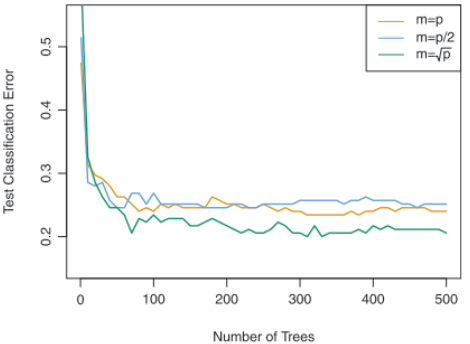
From [JWHT13]

No increase in complexity



From [Smi18]

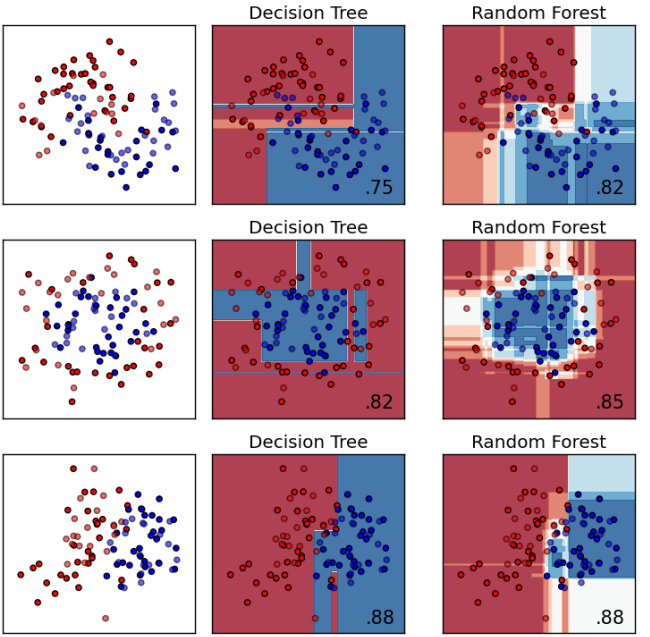
Adding neurons in a NN increases complexity



From [JWHT13]

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

Classification boundaries



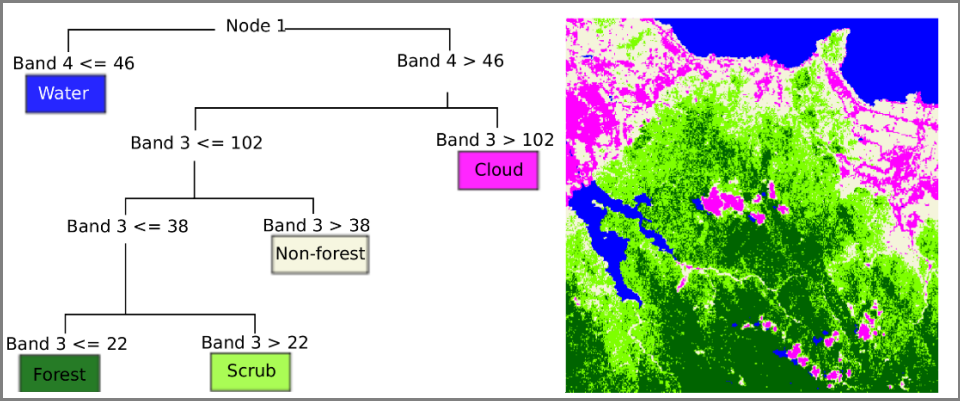
What does the shading represent?

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)
  An option allows deciding whether to use all the dataset to build each tree or a random subset

Boosting

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

Interpretability: Feature Importance

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

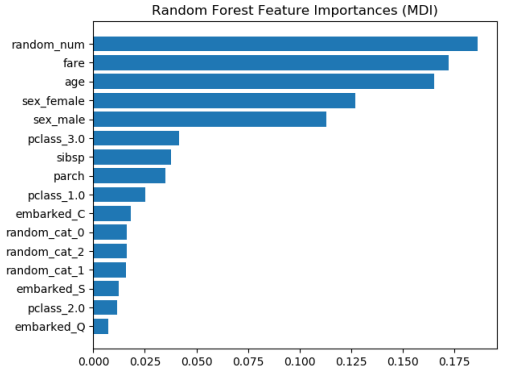
Importance of a feature:[1]

- 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.

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

Interpretability: Feature Importance



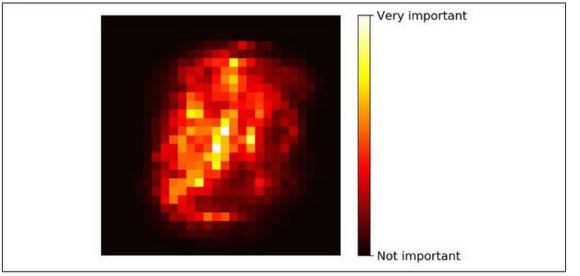


Figure 7-6. MNIST pixel importance (according to a Random Forest classifier)

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)

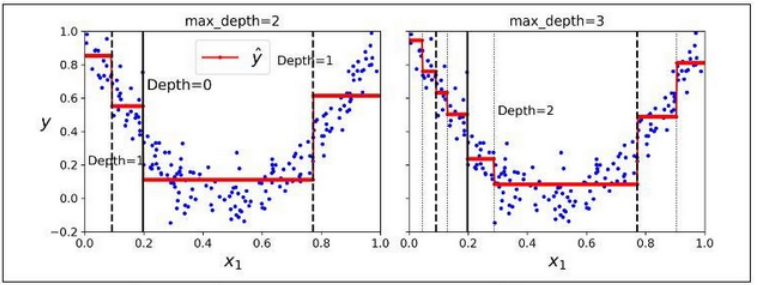


Figure 6-5. Predictions of two Decision Tree regression models

From [Ger19].

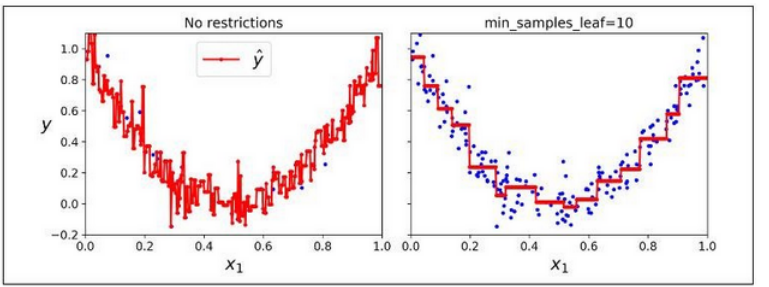


Figure 6-6. Regularizing a Decision Tree regressor

Decision tree

- Training: CART algorithm
- Entropy, Gini inpurity, Information Gain
- Instability

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

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[BK11] Eric Bauer and Ron Kohavi, *An Empirical Comparison of Voting Classification Algorithms : Bagging , Boosting , and Variants*, Machine Learning **38** (2011), no. 1998, 1–38.

[Ger19] Aurelien Geron, *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, O'Reilly, 2019.

[JWHT13] Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani, *An introduction to Statistical Learning*, vol. 7, 2013.

[KPZ+14] 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).

[KS13] Pushmeet Kohli and Jamie Shotton, *Key developments in human pose estimation for kinect*, pp. 63–70, Springer London, London, 2013.

References II

[Smi18] 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.