

INTRO TO DATA SCIENCE LECTURE 12: DECISION TREE CLASSIFIERS

Rob Hall DAT9 SF // September 18, 2014

LAST TIME:

- GITHUB SETUP
- RECOMMENDATION SYSTEMS
- IN-CLASS EXERCISE: BEER RECOMMENDER

QUESTIONS?

I. DECISION TREES
II. BUILDING DECISION TREES
III. OPTIMIZATION FUNCTIONS
IV. PREVENTING OVERFITTING
V. (BRIEF INTRO TO) RANDOM FORESTS

EXERCISE:

V. IMPLEMENTING DECISION TREES WITH SCIKIT-LEARN

I. DECISION TREES

	continuous	categorical
supervised	???	???
unsupervised	???	???

supervisedregressionclassificationunsuperviseddimension reductionclustering

DECISION TREE CLASSIFIERS

Q: What is a decision tree?

- Q: What is a decision tree?
- A: A non-parametric hierarchical classification technique.

Q: What is a decision tree?

A: A non-parametric hierarchical classification technique.

non-parametric: no parameters, no distribution assumptions

Q: What is a decision tree?

A: A non-parametric hierarchical classification technique.

non-parametric: no parameters, no distribution assumptions

hierarchical: consists of a sequence of questions which yield a class label when applied to any record

DECISION TREE CLASSIFIERS

Q: How is a decision tree represented?

DECISION TREE CLASSIFIERS

- Q: How is a decision tree represented?
- A: Using a configuration of nodes and edges.

Q: How is a decision tree represented?

A: Using a configuration of nodes and edges.

More concretely, as a multiway tree, which is a type of (directed acyclic) graph.

Q: How is a decision tree represented?

A: Using a configuration of nodes and edges.

More concretely, as a multiway tree, which is a type of (directed acyclic) graph.

In a decision tree, the nodes represent questions (test conditions) and the edges are the answers to these questions.

TYPES OF NODES

The top node of the tree is called the **root node**. This node has 0 incoming edges, and 2+ outgoing edges.

The top node of the tree is called the **root node**. This node has 0 incoming edges, and 2+ outgoing edges.

An internal node has 1 incoming edge, and 2+ outgoing edges. Internal nodes represent test conditions.

The top node of the tree is called the **root node**. This node has 0 incoming edges, and 2+ outgoing edges.

An internal node has 1 incoming edge, and 2+ outgoing edges. Internal nodes represent test conditions.

A **leaf node** has 1 incoming edge and, 0 outgoing edges. Leaf nodes correspond to class labels.

The top node of the tree is called the **root node**. This node has 0 incoming edges, and 2+ outgoing edges.

An internal node has 1 incoming edge, and 2+ outgoing edges. Internal nodes represent test conditions.

A leaf node has 1 incoming edge and, 0 outgoing edges. L correspond to class labels.

NOTE

The nodes in our tree are connected by directed edges.

These directed edges lead from parent nodes to child nodes.

Table 4.1. The vertebrate data set.

Name	Body	Skin	Gives	Aquatic	Aerial	Has	Hiber-	Class
	Temperature	Cover	Birth	Creature	Creature	Legs	nates	Label
human	warm-blooded	hair	yes	no	no	yes	no	mammal
python	cold-blooded	scales	no	no	no	no	yes	reptile
salmon	cold-blooded	scales	no	yes	no	no	no	fish
whale	warm-blooded	hair	yes	yes	no	no	no	mammal
frog	cold-blooded	none	no	semi	no	yes	yes	amphibian
komodo	cold-blooded	scales	no	no	no	yes	no	reptile
dragon								
bat	warm-blooded	hair	yes	no	yes	yes	yes	mammal
pigeon	warm-blooded	feathers	no	no	yes	yes	no	bird
cat	warm-blooded	fur	yes	no	no	yes	no	mammal
leopard	cold-blooded	scales	yes	yes	no	no	no	fish
shark								
turtle	cold-blooded	scales	no	semi	no	yes	no	reptile
penguin	warm-blooded	feathers	no	semi	no	yes	no	bird
porcupine	warm-blooded	quills	yes	no	no	yes	yes	mammal
eel	cold-blooded	scales	no	yes	no	no	no	fish
salamander	cold-blooded	none	no	semi	no	yes	yes	amphibian

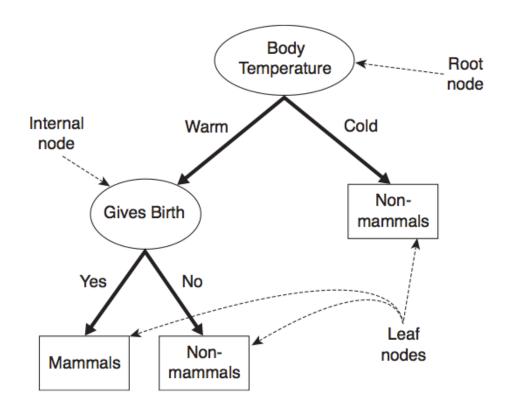


Figure 4.4. A decision tree for the mammal classification problem.

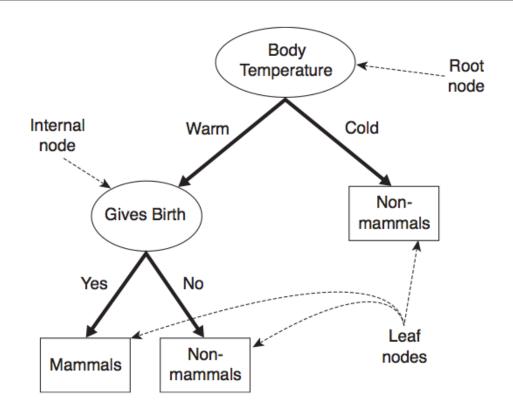


Figure 4.4. A decision tree for the mammal classification problem.

NOTE

Internal nodes represent test conditions which partition the records at that node.

	Name	Body	Skin	Gives	Aquatic	Aerial	Has	Hiber-	Class
		Temperature	Cover	Birth	Creature	Creature	Legs	nates	Label
Γ	gila monster	cold-blooded	scales	no	no	no	yes	yes	?

Now, let's try an example...

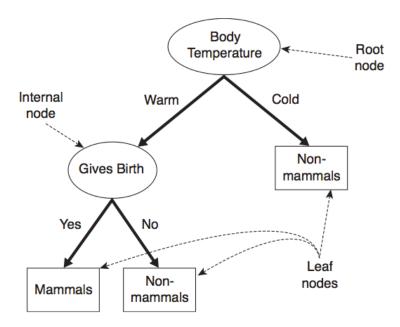


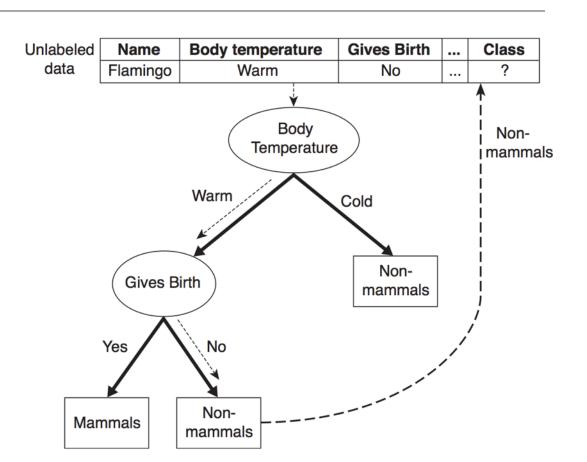
Figure 4.4. A decision tree for the mammal classification problem.

Unlabeled	Name	Bod
data	Flamingo	

1	Name	Body temperature	Gives Birth	 Class
	Flamingo	Warm	No	 ?

And another example...

And another example...



II. BUILDING DECISION TREES

A: One possibility would be to evaluate all possible decision trees (eg, all permutations of test conditions) for a given dataset.

A: One possibility would be to evaluate all possible decision trees (eg, all permutations of test conditions) for a given dataset.

But this is generally too complex to be practical $\rightarrow 0(2^n)$.

A: One possibility would be to evaluate all possible decision trees (eg, all permutations of test conditions) for a given dataset.

But this is generally too complex to be practical $\rightarrow 0(2^n)$.

Q: How do we find a practical solution that works?

A: One possibility would be to evaluate all possible decision trees (eg, all permutations of test conditions) for a given dataset.

But this is generally too complex to be practical $\rightarrow 0(2^n)$.

Q: How do we find a practical solution that works?

A: Use a heuristic algorithm.

The basic method used to build (or "grow") a decision tree is Hunt's algorithm.

The basic method used to build (or "grow") a decision tree is **Hunt's** algorithm.

This is a greedy recursive algorithm that leads to a local optimum.

The basic method used to build (or "grow") a decision tree is **Hunt's** algorithm.

This is a greedy recursive algorithm that leads to a local optimum.

greedy — algorithm makes locally optimal decision at each step recursive — splits task into subtasks, solves each the same way local optimum — solution for a given neighborhood of points

Hunt's algorithm builds a decision tree by recursively partitioning records into smaller & smaller subsets.

Hunt's algorithm builds a decision tree by recursively partitioning records into smaller & smaller subsets.

The partitioning decision is made at each node according to a metric called purity.

Hunt's algorithm builds a decision tree by recursively partitioning records into smaller & smaller subsets.

The partitioning decision is made at each node according to a metric called purity.

A partition is 100% pure when all of its records belong to a single class.

BUILDING A DECISION TREE

Consider a binary classification problem with classes X, Y. Given a set of records D_t at node t, Hunt's algorithm proceeds as follows:

1) If all records in D_t belong to class X, then t is a leaf node corresponding to class X.

1) If all records in D_t belong to class X, then t is a leaf node corresponding to class X.

NOTE

This is the *base case* for the recursive algorithm.

2) If D_t contains records from both classes, then a test condition is created to partition the records further. In this case, t is an internal node whose outgoing edges correspond to the possible outcomes of this test condition.

2) If D_t contains records from both classes, then a test condition is created to partition the records further. In this case, t is an internal node whose outgoing edges correspond to the possible outcomes of this test condition.

These outgoing edges terminate in **child nodes**. A record d in D_t is assigned to one of these child nodes based on the outcome of the test condition applied to d.

3) These steps are then recursively applied to each child node.

3) These steps are then recursively applied to each child node.

NOTE

Decision trees are easy to interpret, but the algorithms to create them are a bit complicated.

A: There are a few ways to do this.

A: There are a few ways to do this.

Test conditions can create binary splits:

A: There are a few ways to do this.

Test conditions can create binary splits:

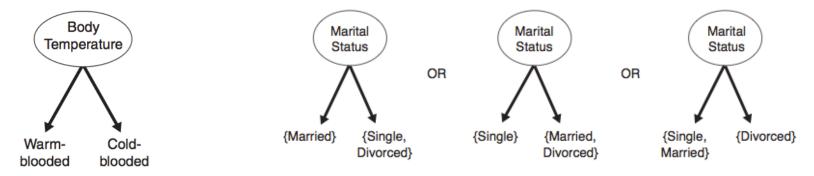
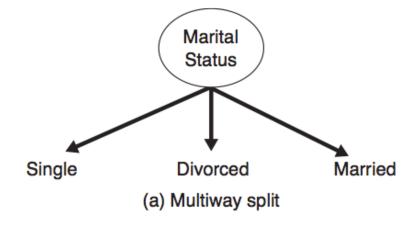


Figure 4.8. Test condition for binary attributes.

(b) Binary split {by grouping attribute values}

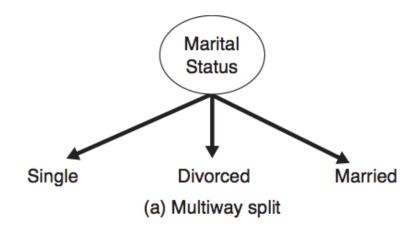
A: There are a few ways to do this.

Alternatively, we can create multiway splits:



A: There are a few ways to do this.

Alternatively, we can create multiway splits:



NOTE

Multiway splits can produce purer subsets, but may lead to overfitting!

- Q: How do we partition the training records?
- A: There are a few ways to do this.

For continuous features, we can use either method:

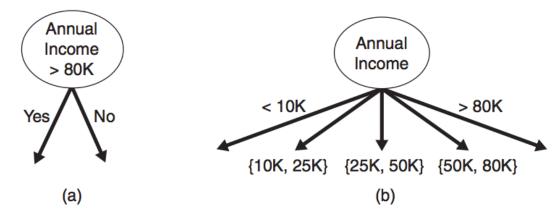


Figure 4.11. Test condition for continuous attributes.

A: There are a few ways to do this.

For continuous features, we can use either method:

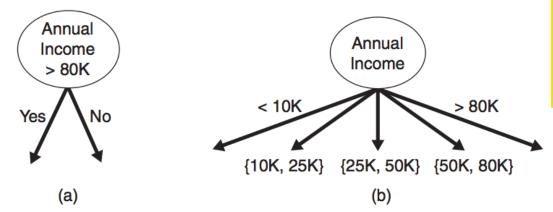


Figure 4.11. Test condition for continuous attributes.

NOTE

There are optimizations that can improve the naïve quadratic complexity of determining the optimum split point for continuous atrributes.

Q: How do we determine the best split?

- Q: How do we determine the best split?
- A: Recall that no split is necessary (at a given node) when all records belong to the same class.

Q: How do we determine the best split?

A: Recall that no split is necessary (at a given node) when all records belong to the same class.

Therefore we want each step to create the partition with the highest possible purity.

Q: How do we determine the best split?

A: Recall that no split is necessary (at a given node) when all records belong to the same class.

Therefore we want each step to create the partition with the highest possible purity.

We need an objective function to optimize!

III. OPTIMIZATION FUNCTIONS

We want our objective function to measure the gain in purity from a particular split.

We want our objective function to measure the gain in purity from a particular split.

Therefore we want it to depend on the class distribution over the nodes (before and after the split).

We want our objective function to measure the gain in purity from a particular split.

Therefore we want it to depend on the class distribution over the nodes (before and after the split).

For example, let p(i I t) be the probability of class i at node t (eg, the fraction of records labeled i at node t).

We are using the frequentist definition of probability here!

We want our objective function to measure the gain in purity from a particular split.

Therefore we want it to depend on the class distribution over the nodes (before and after the split).

For example, let p(i I t) be the probability of class i at not fraction of records labeled i at node t).

Then for a binary (0/1) classification problem,

Then for a binary (0/1) classification problem,

The minimum purity partition is given by the distribution: p(Olt) = p(1lt) = 0.5 Then for a binary (0/1) classification problem,

The minimum purity partition is given by the distribution:

$$p(0|t) = p(1|t) = 0.5$$

The maximum purity partition is given (eg) by the distribution:

$$p(0|t) = 1 - p(1|t) = 1$$

Some measures of impurity include:

Entropy(t) =
$$-\sum_{i=0} p(i|t) \log_2 p(i|t)$$
,

c-1

Gini
$$(t) = 1 - \sum_{i=0}^{3} [p(i|t)]^2$$
,

Classification error(t) =
$$1 - \max_{i}[p(i|t)],$$

Note that each measure achieves its max at 0.5, min at 0 & 1.

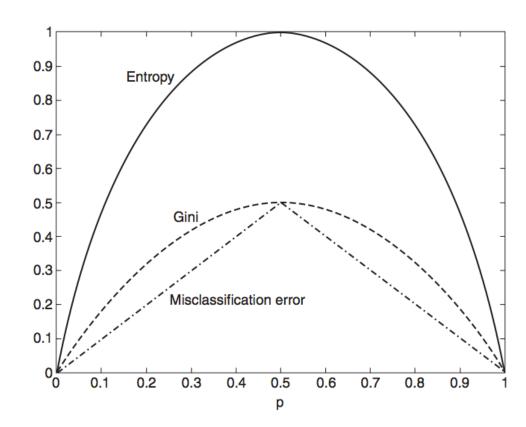


Figure 4.13. Comparison among the impurity measures for binary classification problems.

Note that each measure achieves its max at 0.5, min at 0 & 1.

NOTE

Despite consistency, different measures may create different splits.

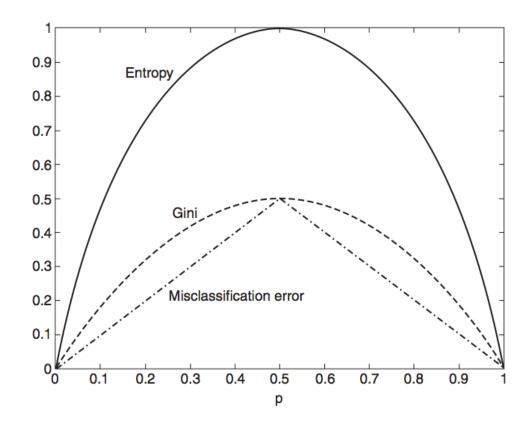


Figure 4.13. Comparison among the impurity measures for binary classification problems.

Impurity measures put us on the right track, but on their own they are not enough to tell us how our split will do.

Impurity measures put us on the right track, but on their own they are not enough to tell us how our split will do.

Q: Why is this true?

Impurity measures put us on the right track, but on their own they are not enough to tell us how our split will do.

Q: Why is this true?

A: We still need to look at impurity before & after the split.

We can make this comparison using the gain:

$$\Delta = I(\text{parent}) - \sum_{\text{children } j} \frac{N_j}{N} I(\text{child } j)$$

We can make this comparison using the gain:

$$\Delta = I(\text{parent}) - \sum_{\text{children } j} \frac{N_j}{N} I(\text{child } j)$$

(Here I is the impurity measure, N_j denotes the number of records at child node j, and N denotes the number of records at the parent node.)

We can make this comparison using the gain:

$$\Delta = I(\text{parent}) - \sum_{\text{children } j} \frac{N_j}{N} I(\text{child } j)$$

(Here I is the impurity measure, N_j denotes the number of records at child node j, and N denotes the number of records at the parent node.)

When I is the entropy, this quantity is called the information gain.

Generally speaking, a test condition with a high number of outcomes can lead to overfitting (ex: a split with one outcome per record).

Generally speaking, a test condition with a high number of outcomes can lead to overfitting (ex: a split with one outcome per record).

One way of dealing with this is to restrict the algorithm to binary splits only (CART).

Generally speaking, a test condition with a high number of outcomes can lead to overfitting (ex: a split with one outcome per record).

One way of dealing with this is to restrict the algorithm to binary splits only (CART).

Another way is to use a splitting criterion which explicitly penalizes the number of outcomes (C4.5)

We can use a function of the information gain called the gain ratio to explicitly penalize high numbers of outcomes:

gain ratio =
$$\frac{\Delta_{info}}{-\sum p(v_i)log_2p(v_i)}$$

(Where $p(v_i)$ refers to the probability of label i at node v)

We can use a function of the information gain called the gain ratio to explicitly penalize high numbers of outcomes:

gain ratio =
$$\frac{\Delta_{info}}{-\sum p(v_i)log_2p(v_i)}$$

This is a form of regularization!

NOTE

(Where $p(v_i)$ refers to the probability of label i at node v)

IV. PREVENTING OVERFITTING

In addition to determining splits, we also need a stopping criterion to tell us when we're done.

In addition to determining splits, we also need a stopping criterion to tell us when we're done.

For example, we can stop when all records belong to the same class, or when all records have the same attributes.

In addition to determining splits, we also need a stopping criterion to tell us when we're done.

For example, we can stop when all records belong to the same class, or when all records have the same attributes.

This is correct in principle, but would likely lead to overfitting.

One possibility is **pre-pruning**, which involves setting a minimum threshold on the gain, and stopping when no split achieves a gain above this threshold.

One possibility is **pre-pruning**, which involves setting a minimum threshold on the gain, and stopping when no split achieves a gain above this threshold.

This prevents overfitting, but is difficult to calibrate in practice (may preserve bias!)

Alternatively we could build the full tree, and then perform pruning as a post-processing step.

Alternatively we could build the full tree, and then perform pruning as a post-processing step.

To prune a tree, we examine the nodes from the bottom-up and simplify pieces of the tree (according to some criteria).

Complicated subtrees can be replaced either with a single node, or with a simpler (child) subtree.

V. RANDOM FORESTS

RANDOM FORESTS

A random forest is an ensemble of decision trees where each base classifier is grown using a random effect.

A random forest is an ensemble of decision trees where each base classifier is grown using a random effect.

One way to do this is to randomly choose one of the top k features to split each node.

A random forest is an ensemble of decision trees where each base classifier is grown using a random effect.

One way to do this is to randomly choose one of the top k features to split each node.

For a small number of features, we can also create linear combinations of features and select splits from the enhanced feature set (Forest-RC).

A random forest is an ensemble of decision trees where each base classifier is grown using a random effect.

One way to do this is to randomly choose one of the top k features to split each node.

For a small number of features, we can also create linear combinations of features and select splits from the enhanced feature set (Forest-RC).

Or, we can select splitting features completely at random (Forest-RI).

EX: DECISION TREES IN PYTHON