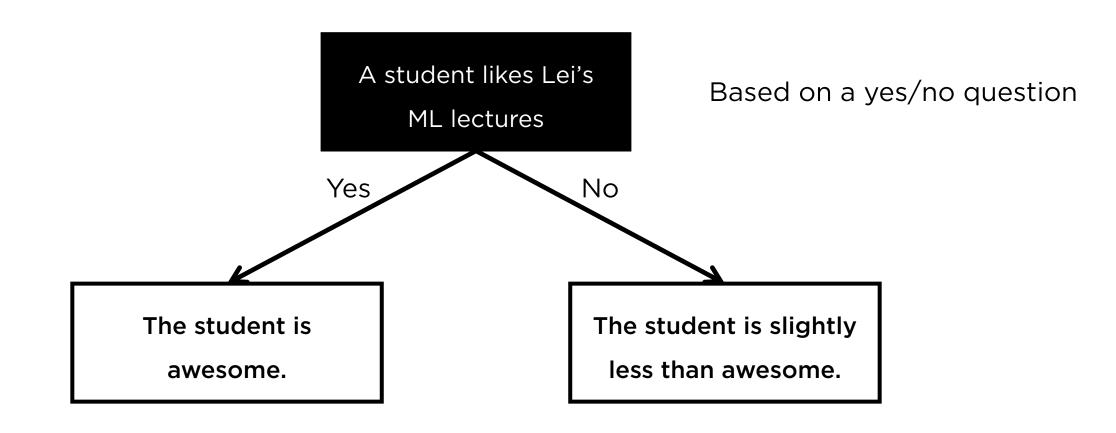
# Machine Learning

Lecture 6 - Decision Trees and Random Forests

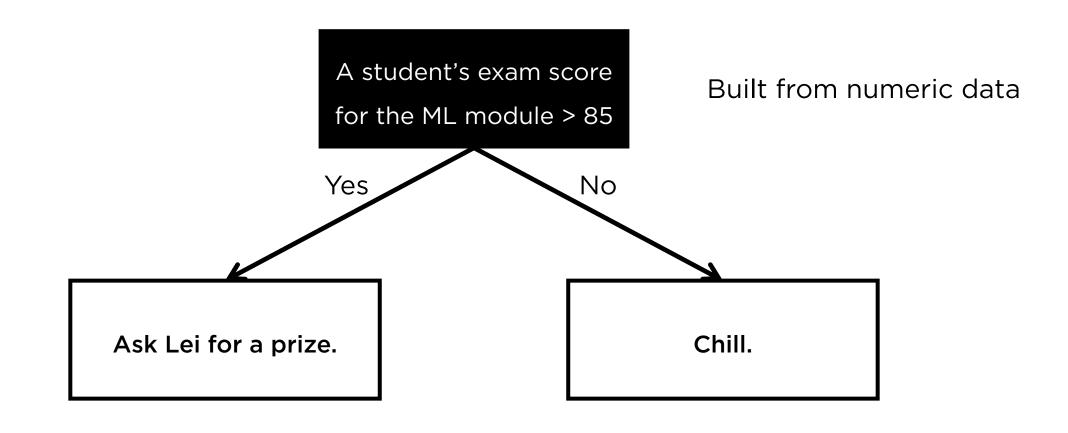
Dr SHI Lei



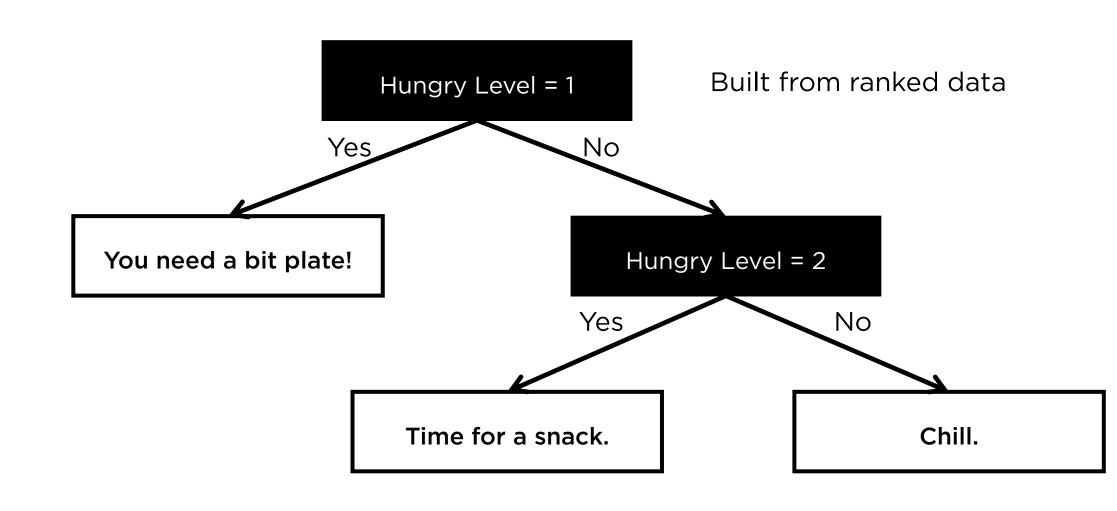
An example



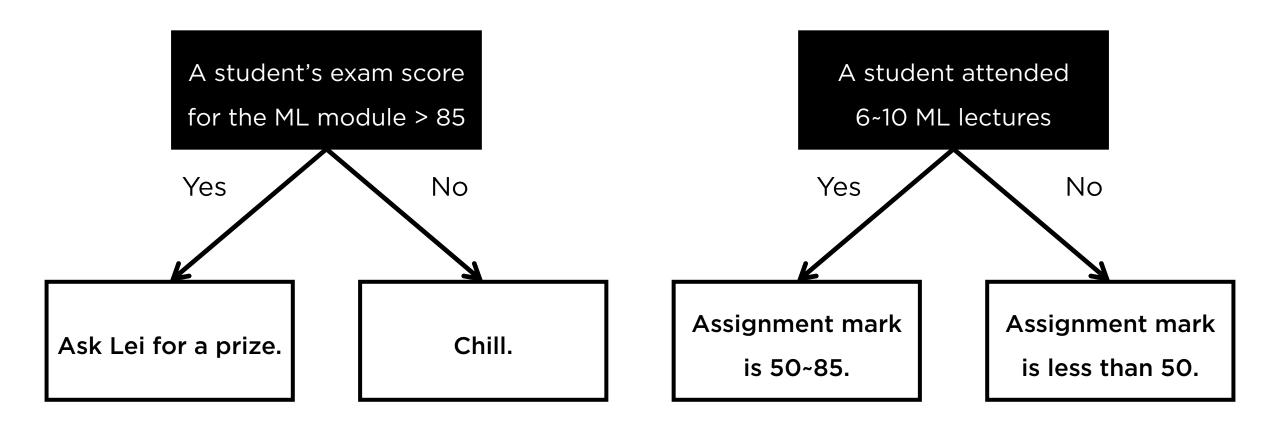
Another example



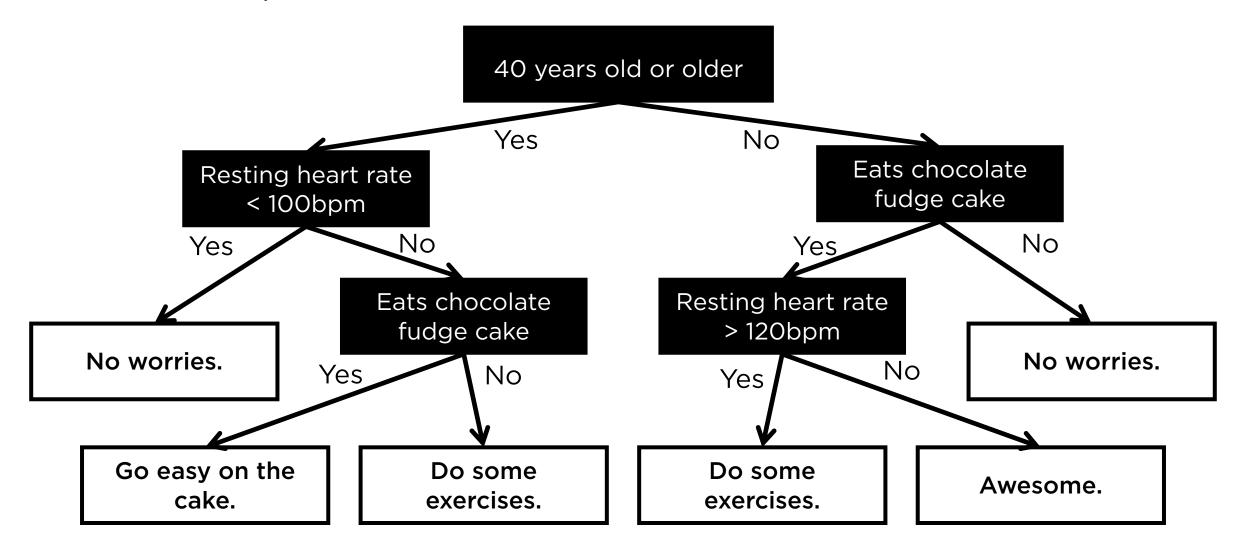
One more example

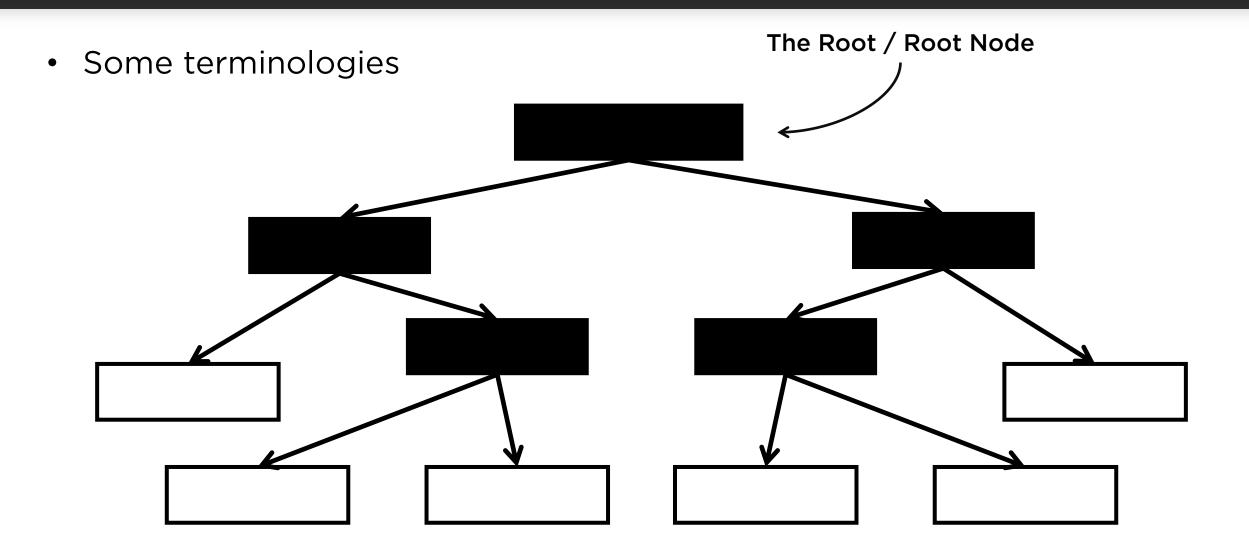


The classification can be Categorical or Numerical

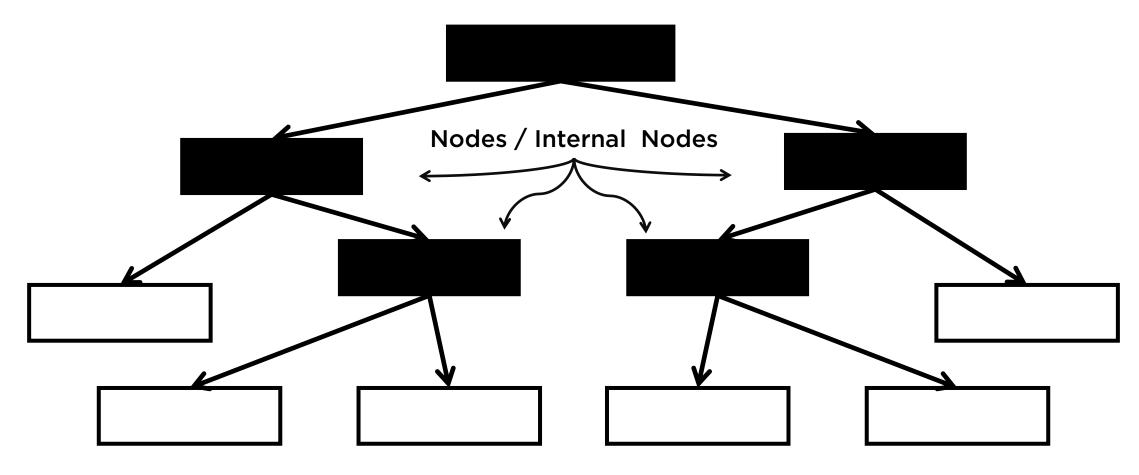


A more complicated decision tree

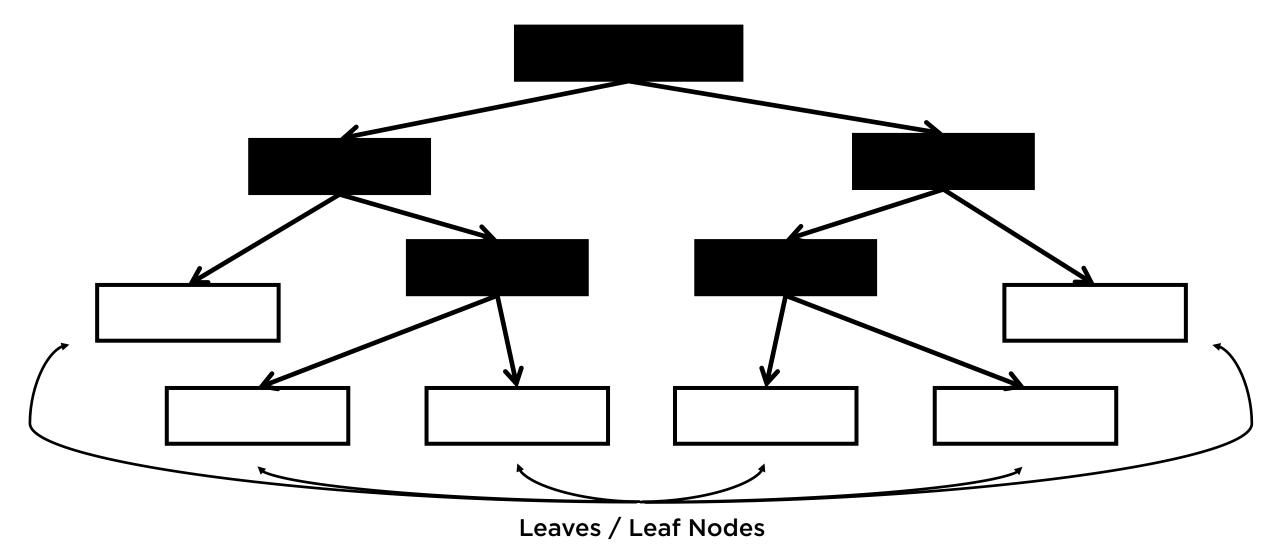




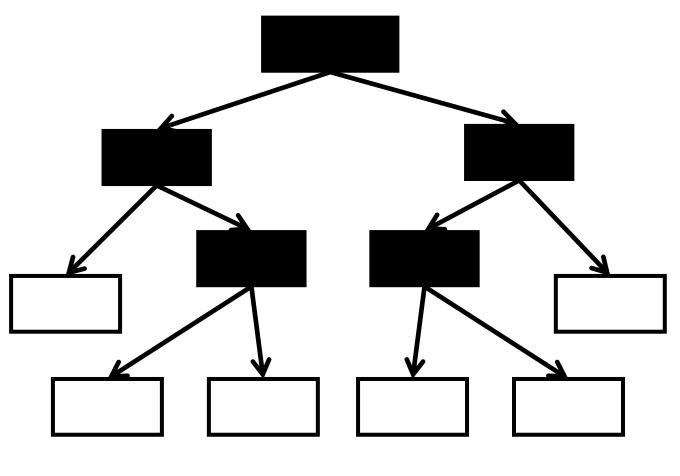
Some terminologies



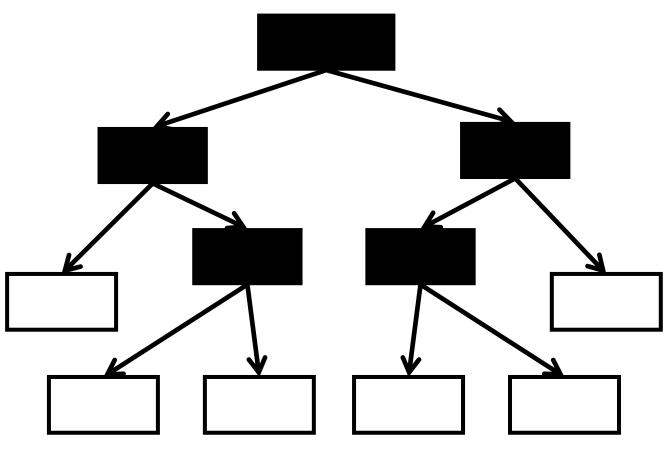
Some terminologies



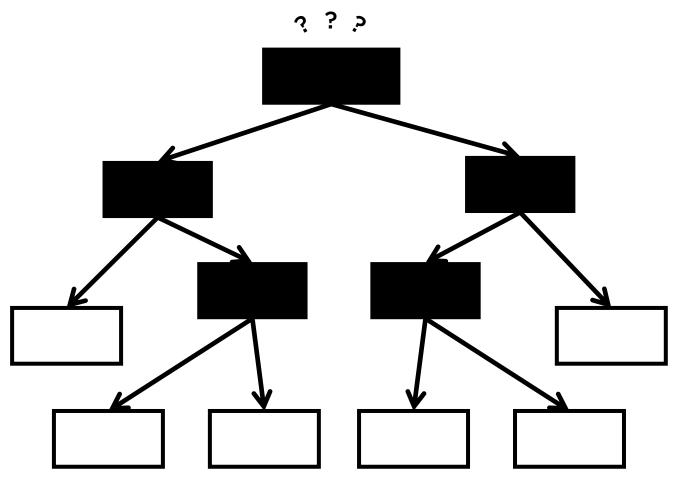
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Š	Yes



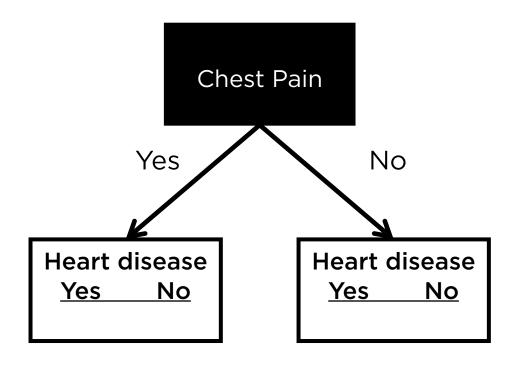
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes



Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Ş	Yes



Good blood circulation	Blocked arteries	Heart disease
No	No	No
Yes	Yes	Yes
Yes	No	No
No	?	Yes
	blood circulation  No  Yes  Yes  No	blood circulationBlocked arteriesNoNoYesYesYesNoNo?



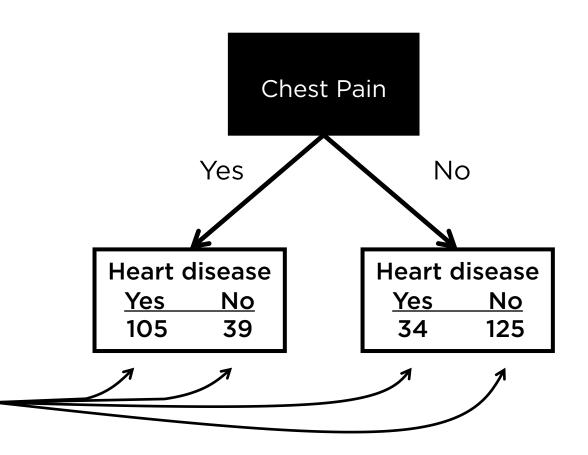
Chest pain	Good blood circulation	Blocked arteries	Heart disease	
No	No	No	No	Chest Pain
Yes	Yes	Yes	Yes	Yes No
Yes	Yes	No	No	Heart disease Heart disease
Yes	No	?	Yes	Yes No Yes No

Chest pain	Good blood circulation	Blocked arteries	Heart disease	
No	No	No	No	Chest Pain
Yes	Yes	Yes	Yes	Yes No
Yes	Yes	No	No	Heart disease Heart disease
Yes	No	?	Yes	<u>Yes No</u> <u>Yes No</u> 1

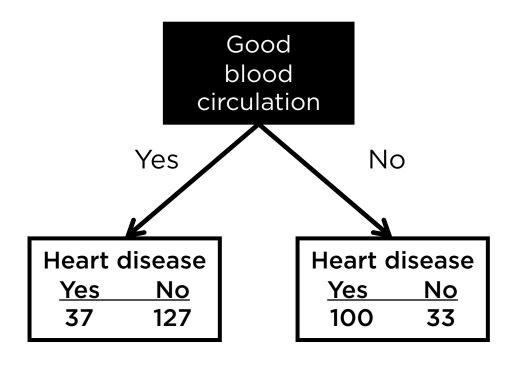
Chest pain	Good blood circulation	Blocked arteries	Heart disease	
No	No	No	No	Chest Pain
Yes	Yes	Yes	Yes	Yes No
Yes	Yes	No	No	Heart disease Heart disease
Yes	No	?	Yes	Yes No 1 1 1 1
***				

Chest pain	Good blood circulation	Blocked arteries	Heart disease	
No	No	No	No	Chest Pain
Yes	Yes	Yes	Yes	Yes No
Yes	Yes	No	No	Heart disease Heart disease
Yes	No	?	Yes	Yes         No           2         1             Yes         No           1

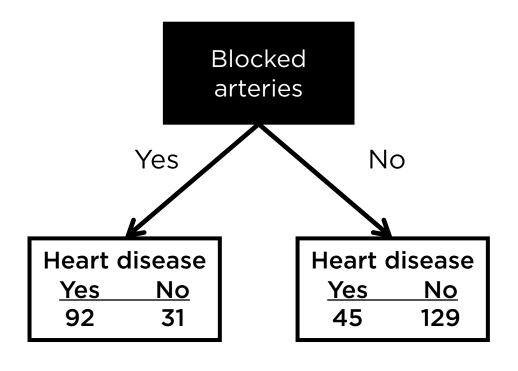
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes



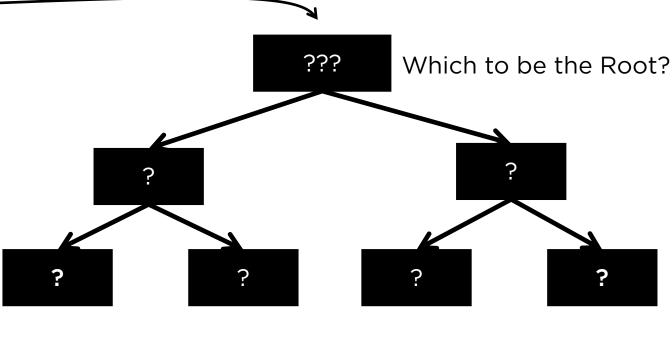
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes



Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	è.	Yes

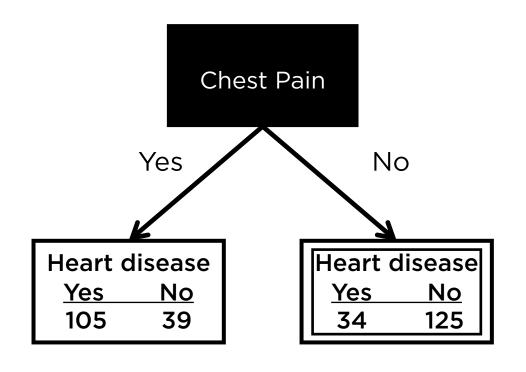


Chest pain	Good blood circulation	Blocked arteries	Heart disease	
No	No	No	No	
Yes	Yes	Yes	Yes	
Yes	Yes	No	No	
Yes	No	?	Yes	



From a raw table of data to a decision tree

Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes

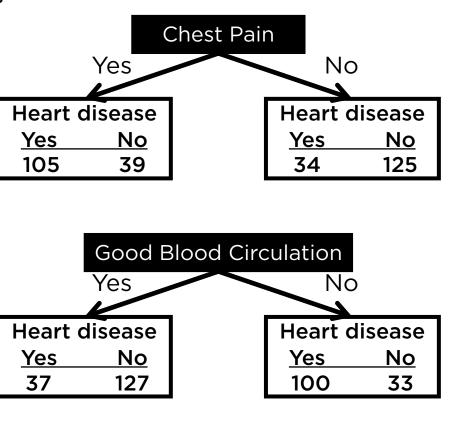


None of the leaf nodes are 100% "Yes Heart Disease" or 100% "No Heart Disease".

They are considered **Impure**.

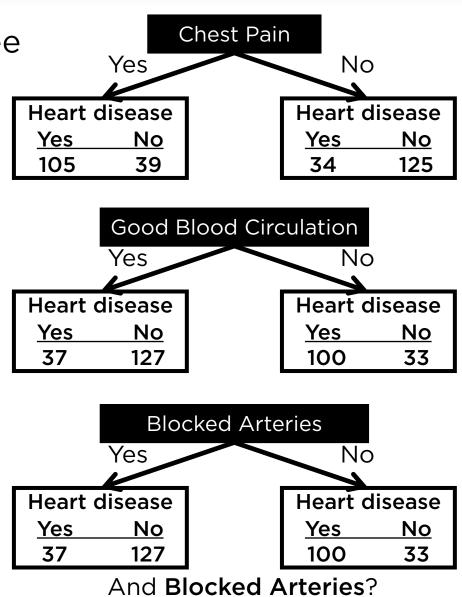
From a raw table of data to a decision tree

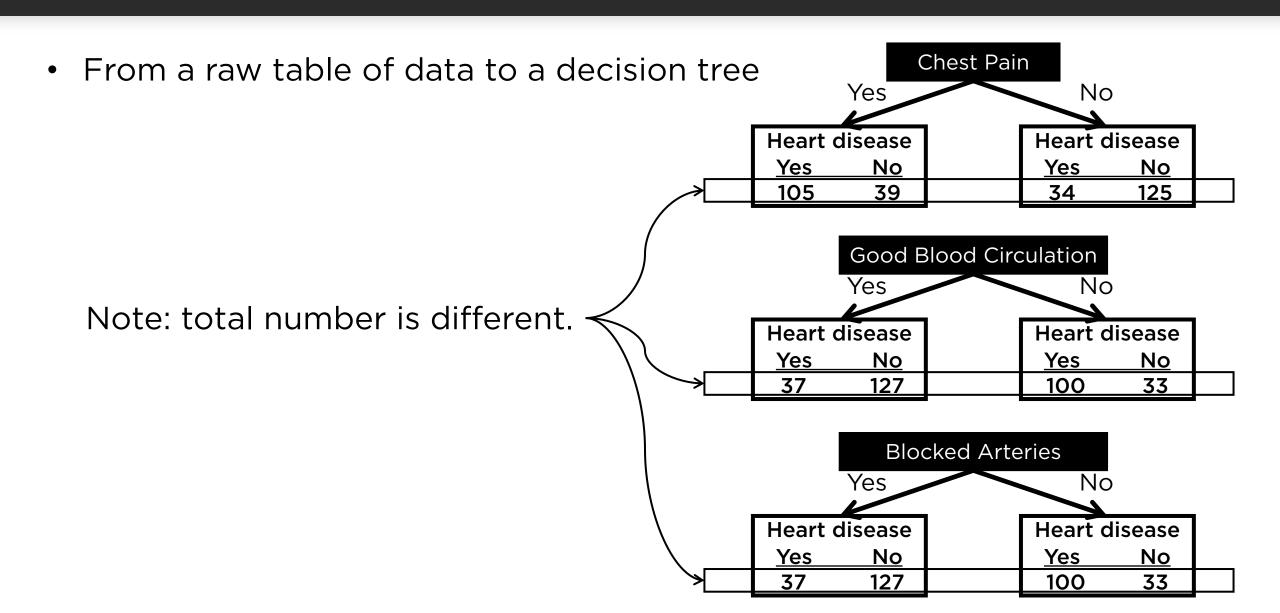
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes



How about **Good Blood Circulation**?

Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Ş	Yes

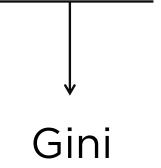


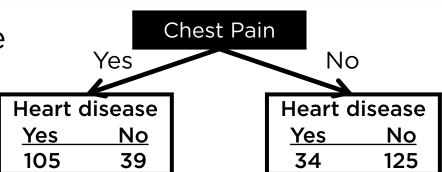


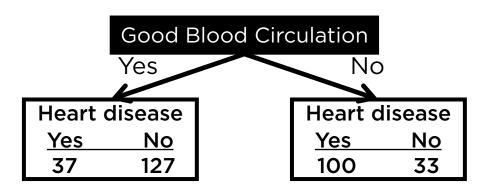
From a raw table of data to a decision tree

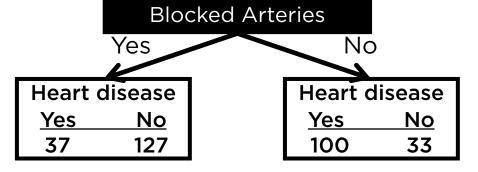
How to decide which is the best?

By measuring and comparing Impurity.

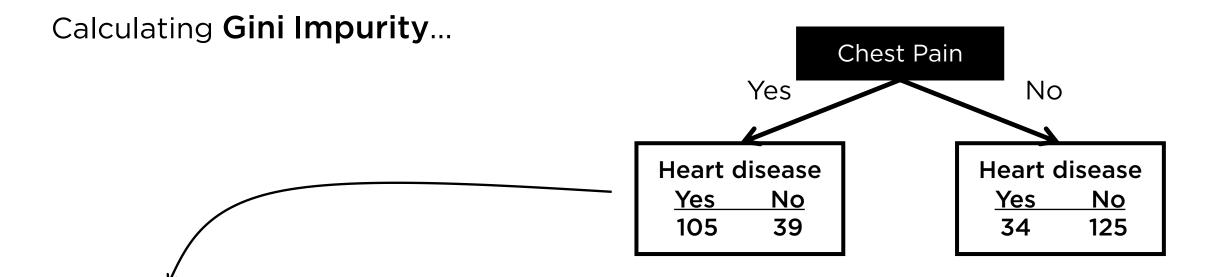








From a raw table of data to a decision tree



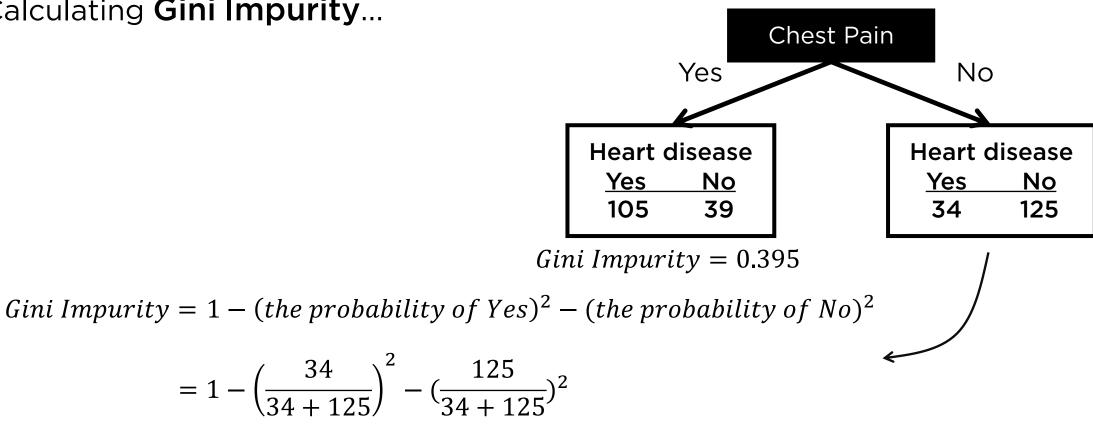
Gini Impurity =  $1 - (the \ probability \ of \ Yes)^2 - (the \ probability \ of \ No)^2$ 

$$= 1 - \left(\frac{105}{105 + 39}\right)^2 - \left(\frac{39}{105 + 39}\right)^2$$
$$= 0.395$$

From a raw table of data to a decision tree

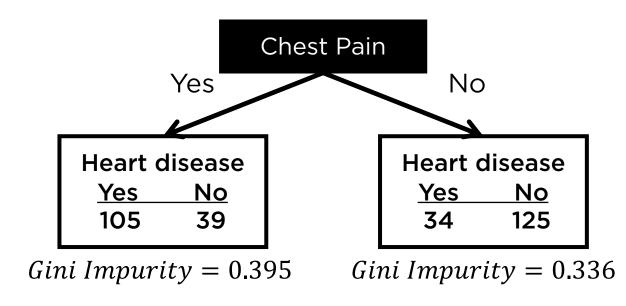


= 0.336



From a raw table of data to a decision tree

Calculating **Gini Impurity**...



 $Gini\ Impurity for\ Chest\ Pain = weighted\ average\ of\ Gini\ impurities\ for\ the\ leaf\ nodes$ 

$$= \frac{144}{144 + 159} \times 0.395 + \frac{159}{144 + 159} \times 0.336$$
$$= 0.364$$

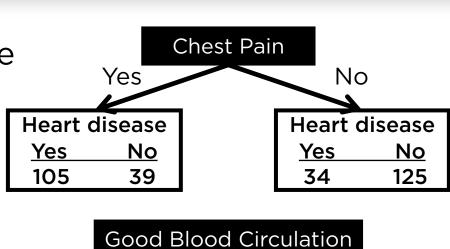
From a raw table of data to a decision tree

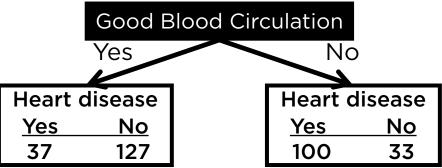
Calculating **Gini Impurity**...

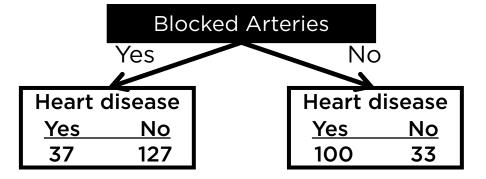
Gini Impurity for Chest Pain = 0.364



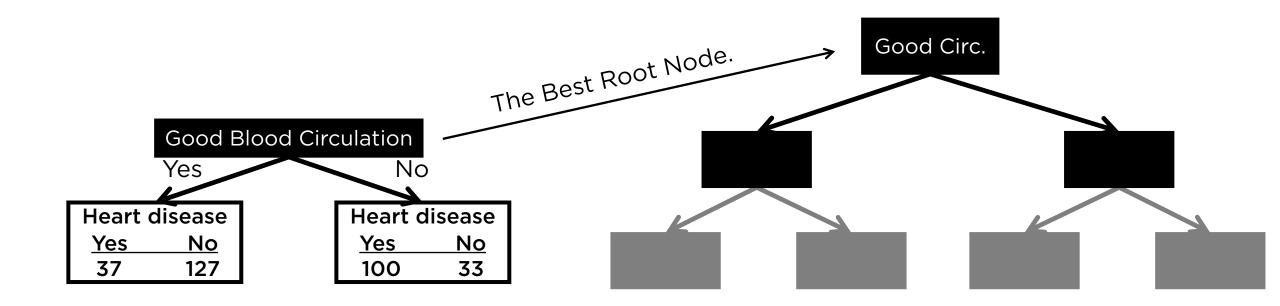
Gini Impurity for **Blocked Arteries** = 0.381

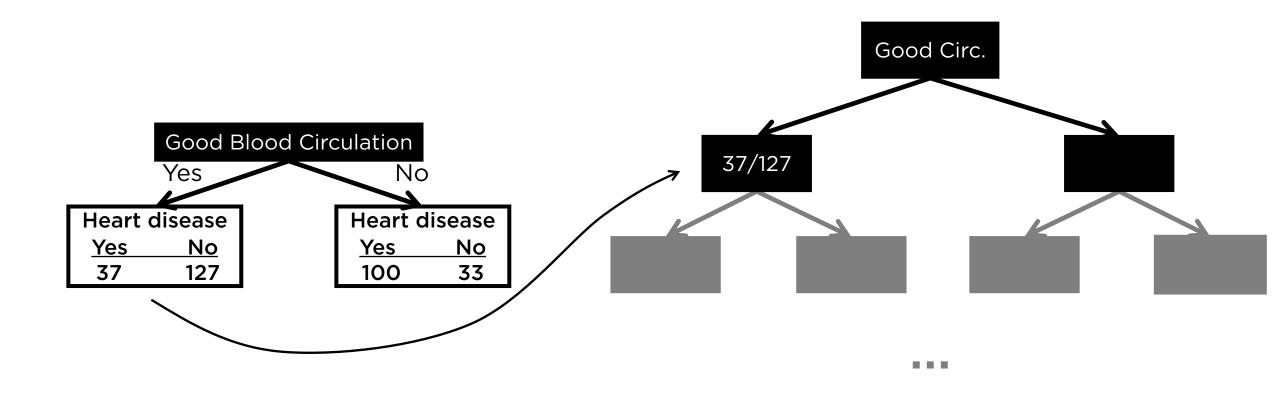


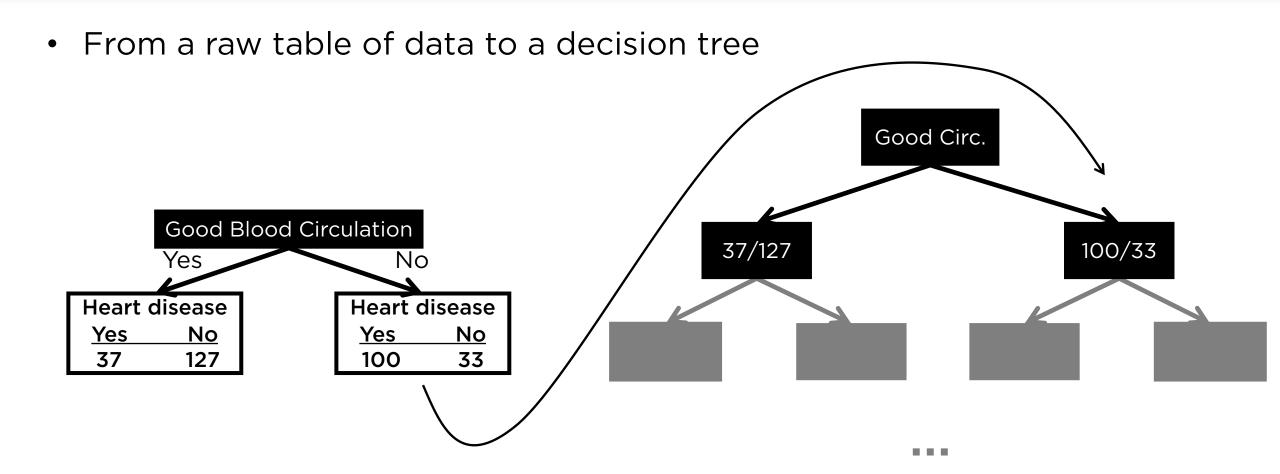




From a raw table of data to a decision tree

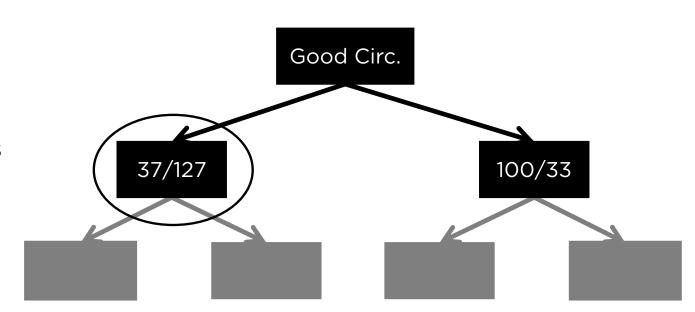






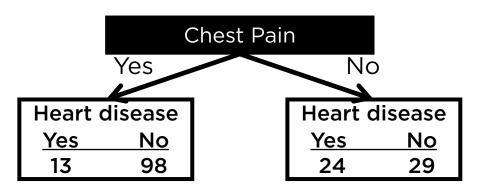
From a raw table of data to a decision tree

How well **Chest Pain** and **Blocked Arteries** separate these 164 patients?

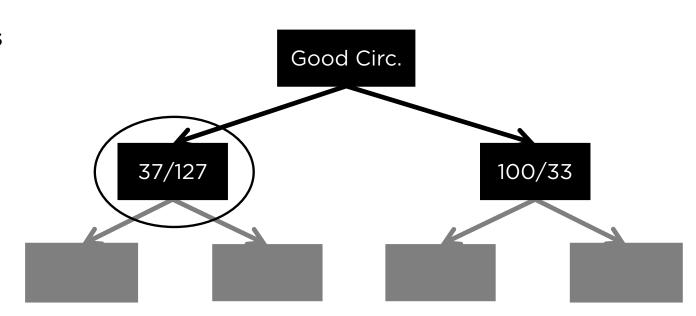


From a raw table of data to a decision tree

How well **Chest Pain** and **Blocked Arteries** separate these 164 patients?

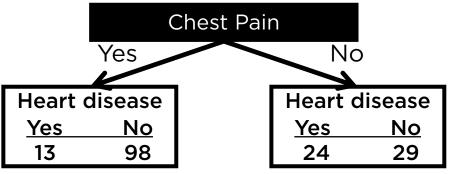


Gini Impurity for Chest Pain = 0.3

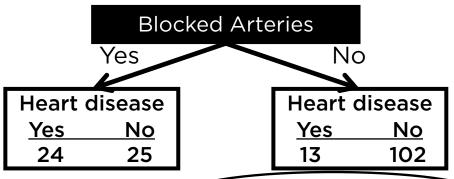


From a raw table of data to a decision tree

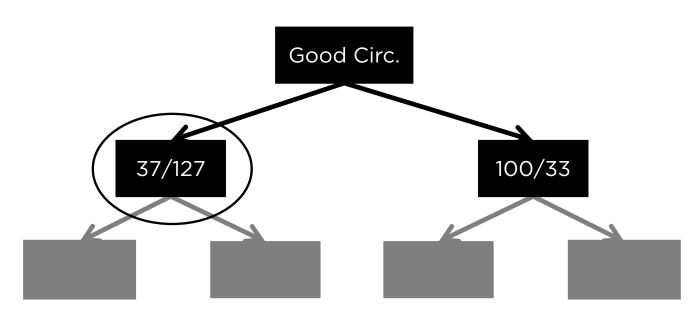
How well **Chest Pain** and **Blocked Arteries** separate these 164 patients?



Gini Impurity for Chest Pain = 0.3

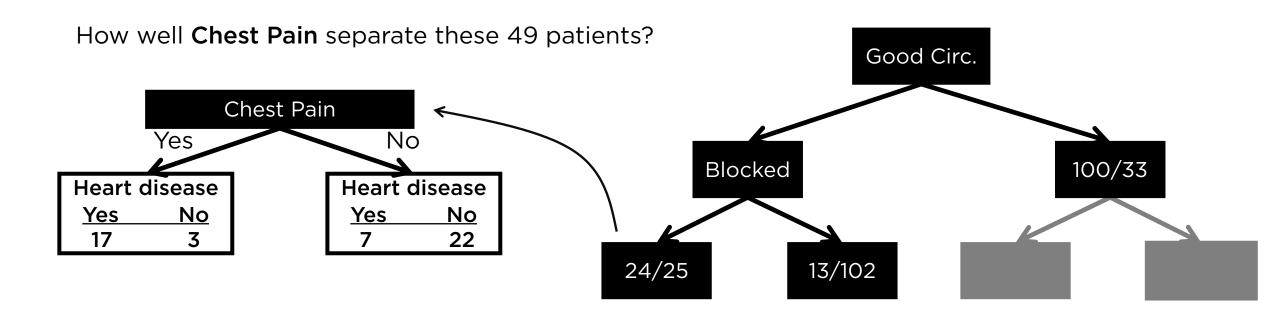


Gini Impurity for **Blocked A**rteries = 0.290

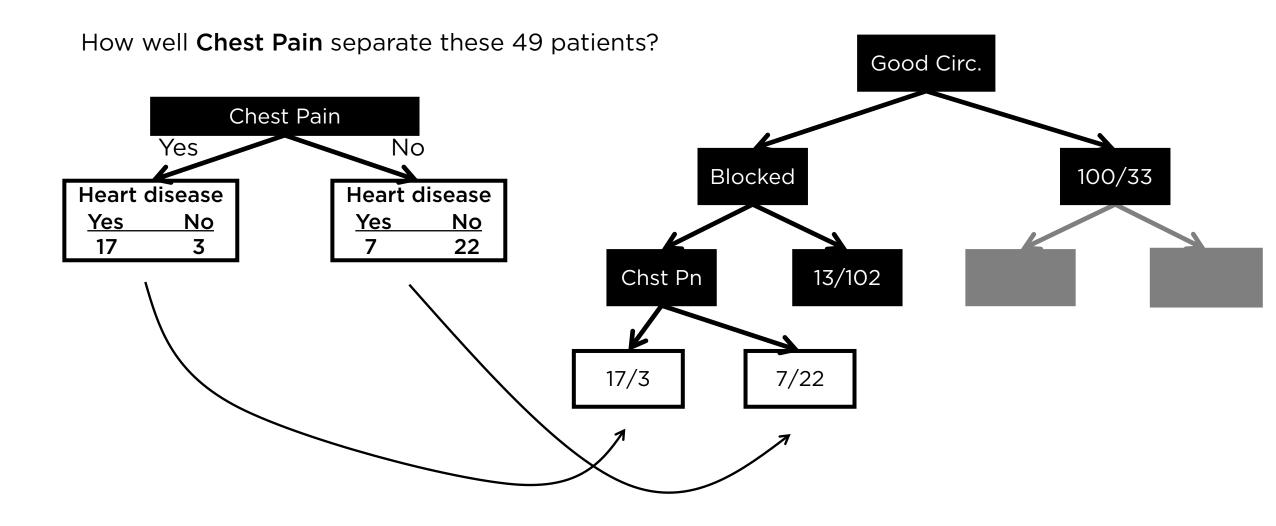


The lowest impurity

From a raw table of data to a decision tree



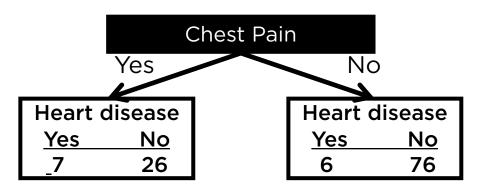
From a raw table of data to a decision tree



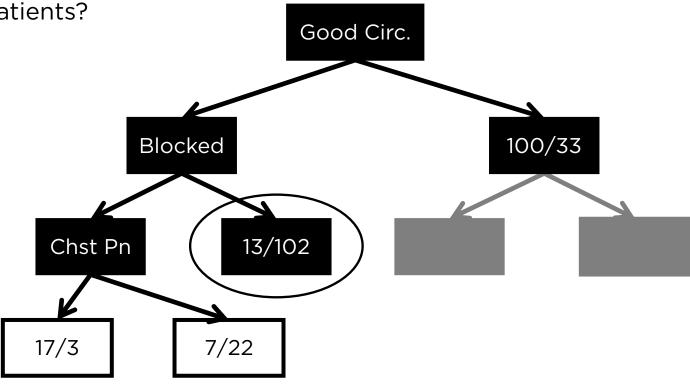
From a raw table of data to a decision tree

How well **Chest Pain** separate these 115 patients?

**Note**: the vast majority of the patients in this node (89%) don't have heart disease.



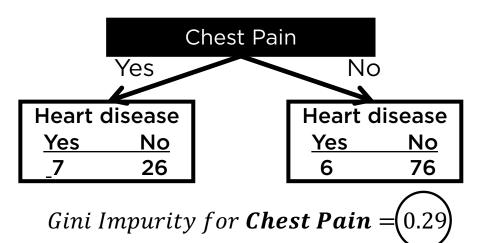
Do these new leaves separate patients better than before?



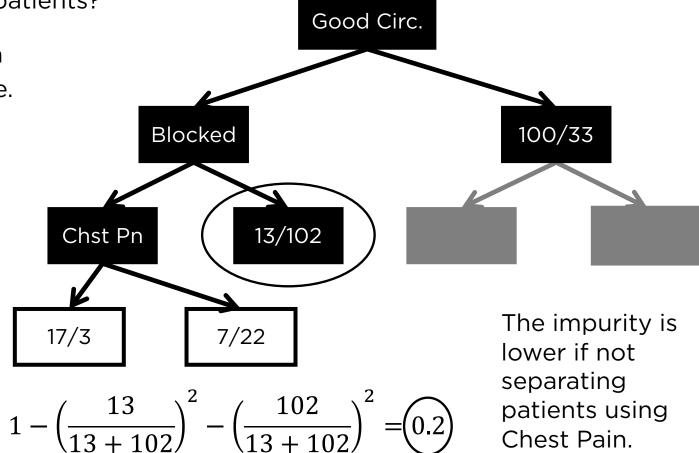
From a raw table of data to a decision tree

How well **Chest Pain** separate these 115 patients?

**Note**: the vast majority of the patients in this node (89%) don't have heart disease.



Gini impurity for this node, before using **Chest Pain** to separate patients is...



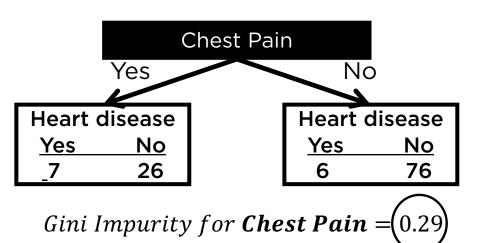
patients using

Chest Pain.

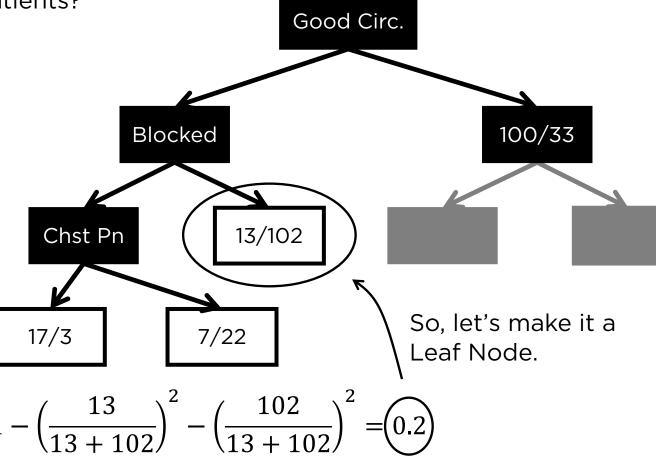
From a raw table of data to a decision tree



**Note**: the vast majority of the patients in this node (89%) don't have heart disease.



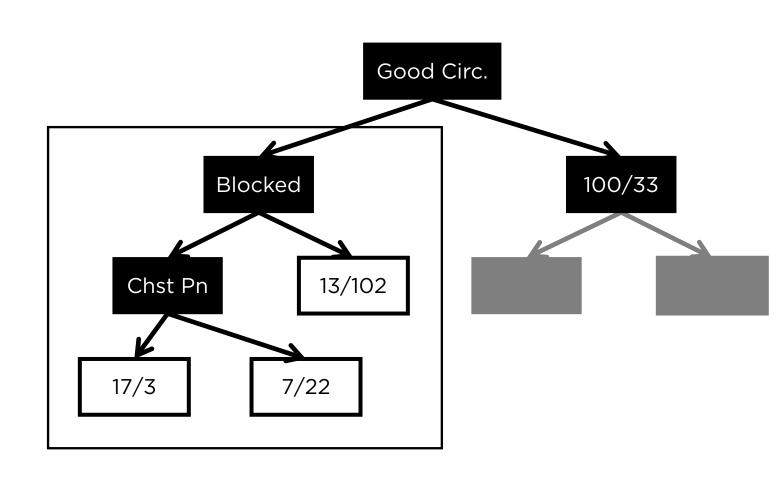
Gini impurity for this node, before using **Chest Pain** to separate patients is...



From a raw table of data to a decision tree



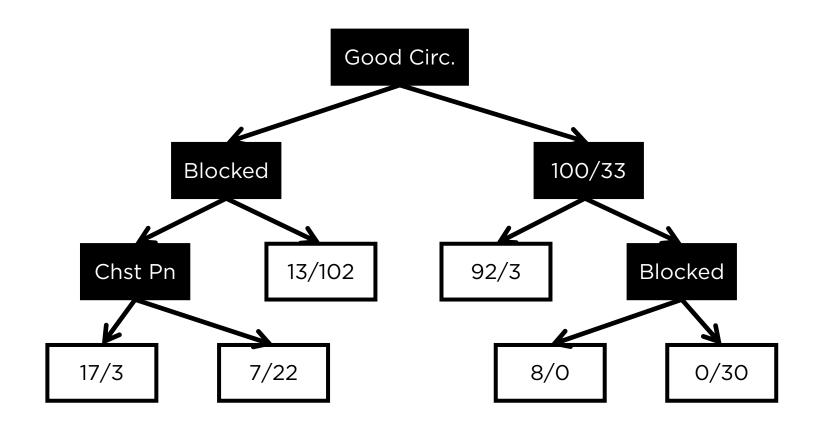
Left side of the Tree completed!



From a raw table of data to a decision tree

Following the exact same steps: Good Circ. 1. Calculate all of the Gini impurity values. 2. If the node itself has the lowest value. Blocked 100/33 leave it as a Leaf node. 3. If separating the data results in an Chst Pn 13/102 improvement, then pick the separation with the lowest Gini impurity value. 17/3 7/22

From a raw table of data to a decision tree



Numeric Data?

• Built tree from Numeric Data

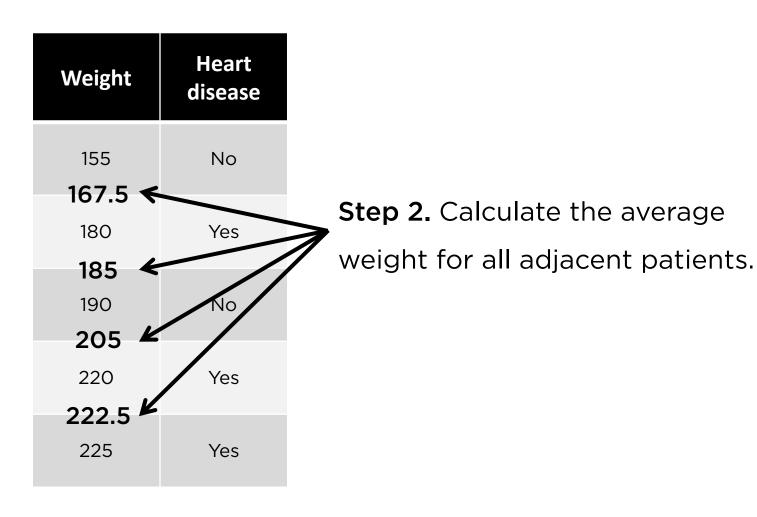
Weight	Heart disease
220	Yes
180	Yes
225	Yes
190	No
155	No

Built tree from Numeric Data



**Step 1.** Sort patients by weight, lowest to highest.

Built tree from Numeric Data

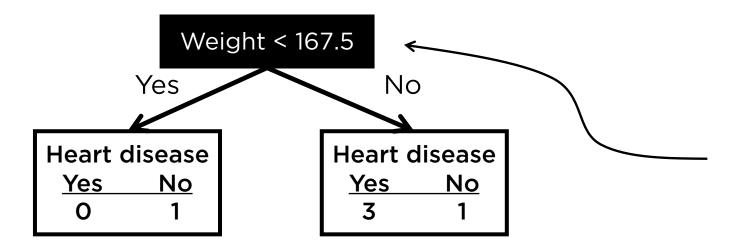


Built tree from Numeric Data

	Weight	Heart disease
Gini impurity? ←	155 <b>— 167.5</b>	No
	180	Yes
Gini impurity? <b>←</b>	<b>- 185</b>	No
Gini impurity? <b>←</b>	<b>– 205</b> 220	Yes
Gini impurity? <b>←</b>	<b>- 222.5</b> 225	Yes

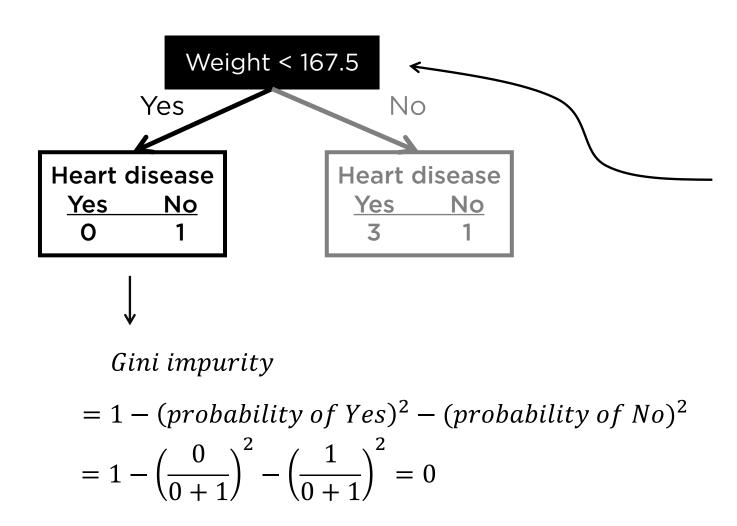
**Step 3.** Calculate the impurity values for each average weight.

• Built tree from Numeric Data



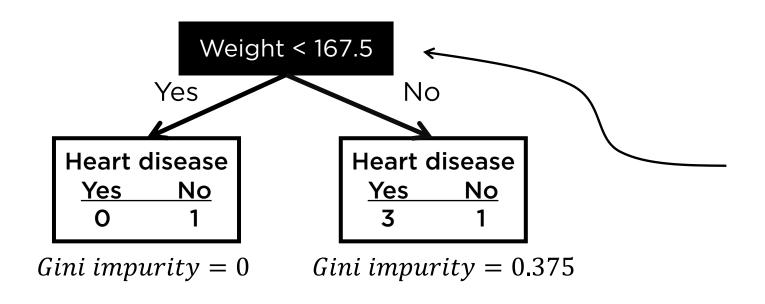
Weight	Heart disease
155	No
<b>167.5</b> 180	Yes
<b>185</b> 190	No
<b>205</b> 220	Yes
<b>222.5</b> 225	Yes

Built tree from Numeric Data



Weight	Heart disease	
155	No	
180	Yes	
185		
190	No	
205		
220	Yes	
	res	
222.5		
225	Yes	

Built tree from Numeric Data

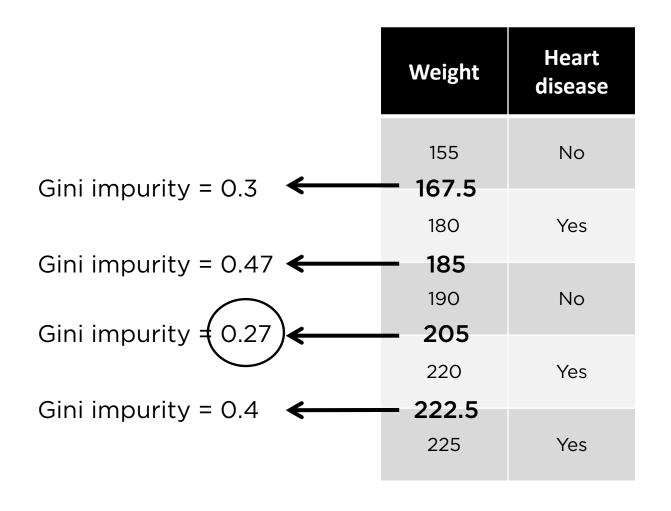


 $Gini\ impurity\ for\ Weight < 167.5$ 

$$= \frac{1}{1+4} \times 0 + \frac{4}{1+4} \times 0.336 = 0.3$$

Weight	Heart disease
155	No
180	Yes
185 190	No
<b>205</b> 220	Yes
<b>222.5</b> 225	Yes

#### Built tree from Numeric Data

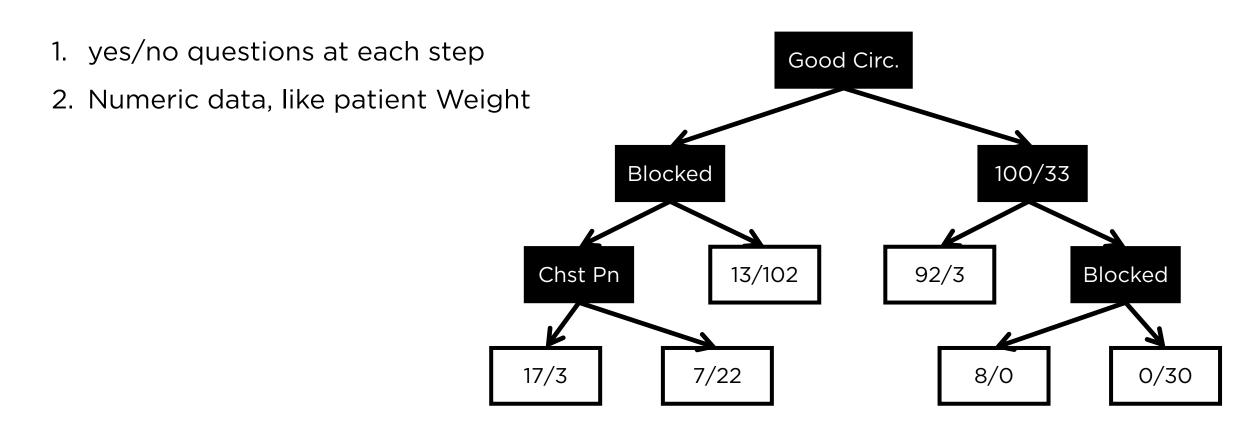


**Step 3.** Calculate the impurity values for each average weight.

The lowest impurity occurs when using Weight < 205.

This is the cutoff to use when comparing Weight to Chest Pain, or Blocked Arteries.

To build a tree



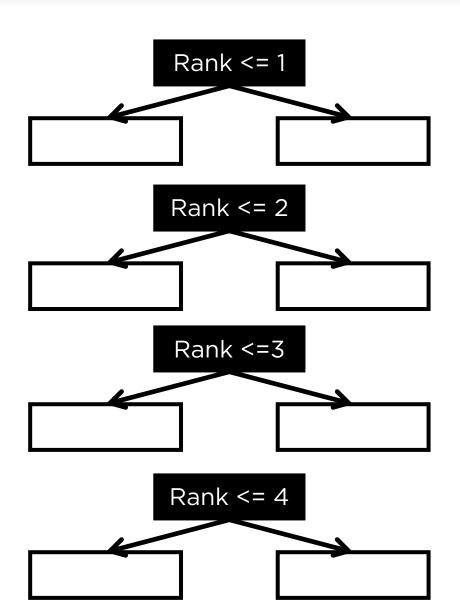
Ranked Data & Multiple Choice Data?

Built tree from Ranked Data

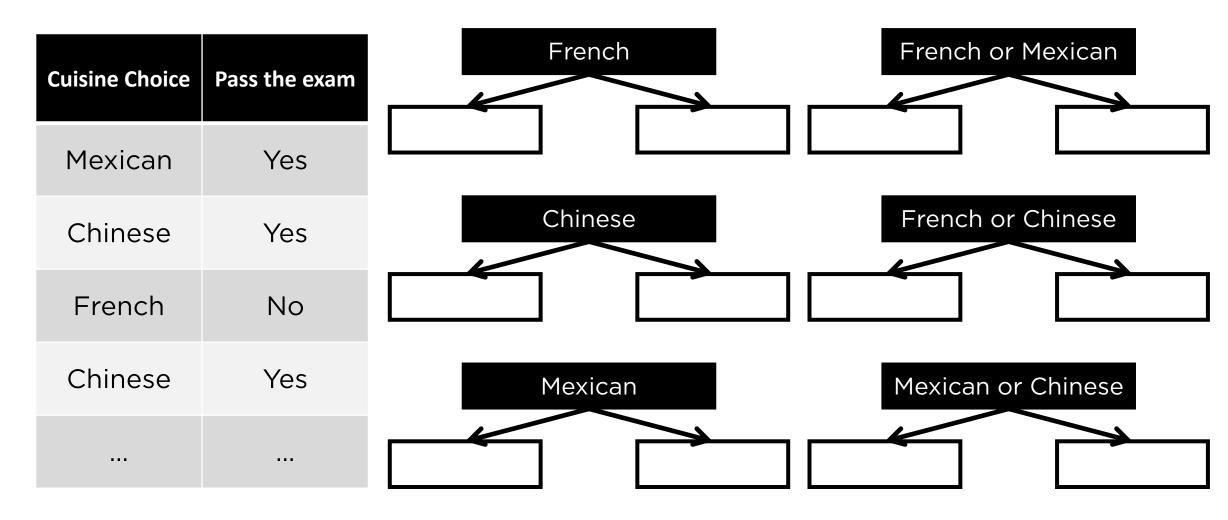
Rank my ML lectures	Pass the exam
2	No
5	Yes
4	Yes
3	No

Built tree from Ranked Data

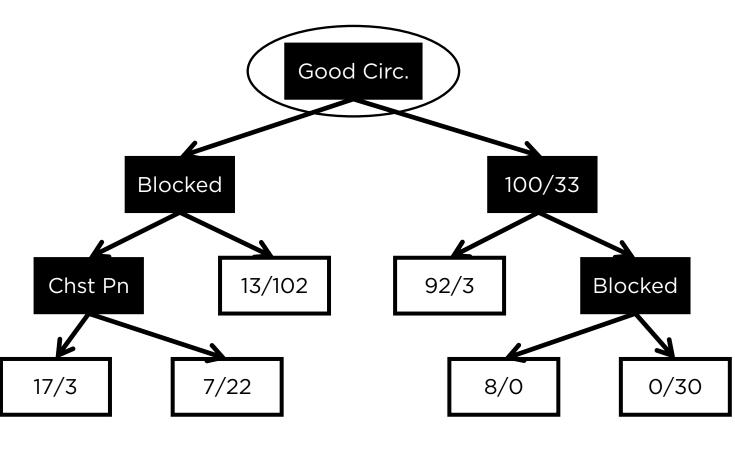
Rank my ML lectures	Pass the exam
2	No
5	Yes
4	Yes
3	No
	•••



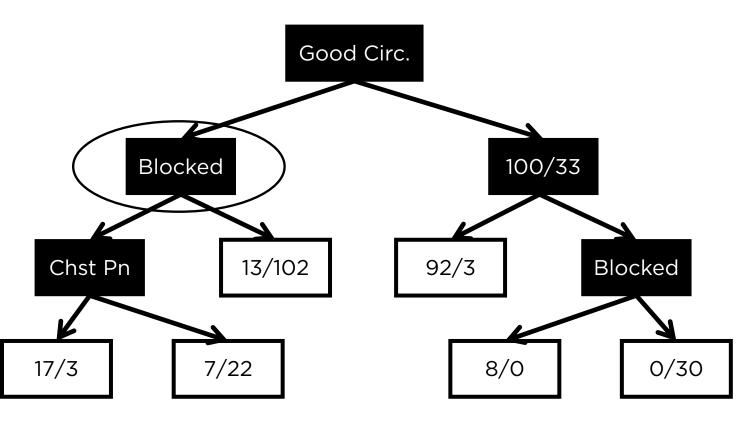
• Built tree from Multiple Choices Data



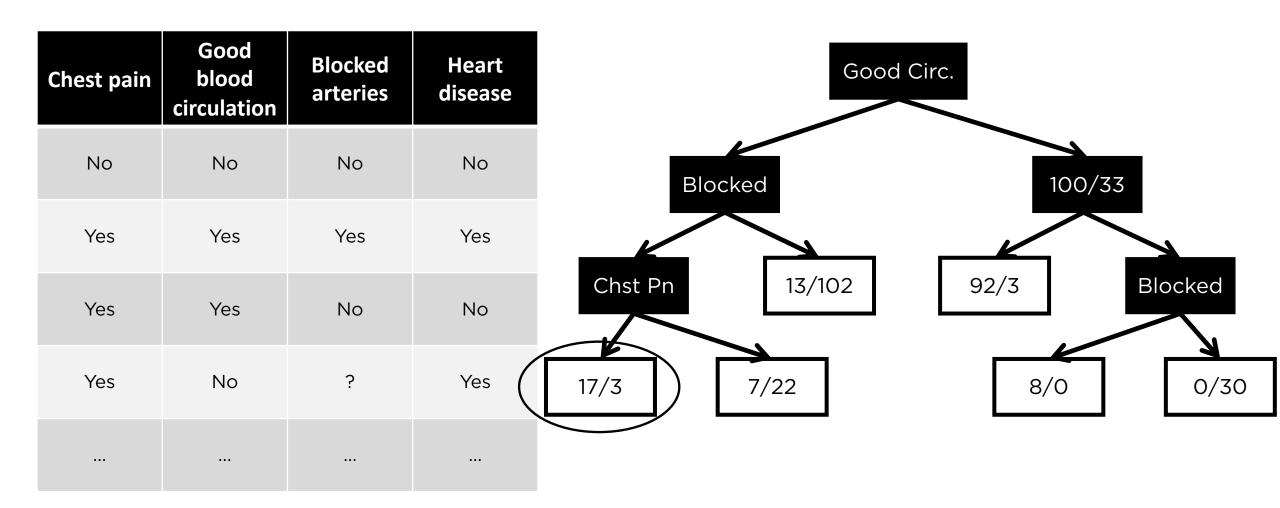
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Ś	Yes
		***	



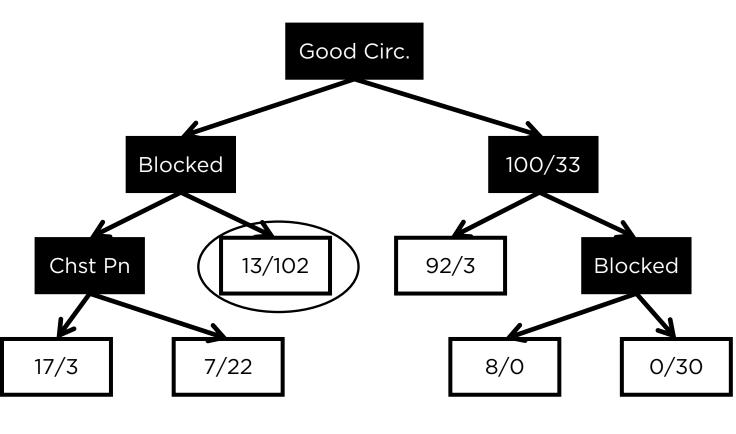
Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Ş	Yes

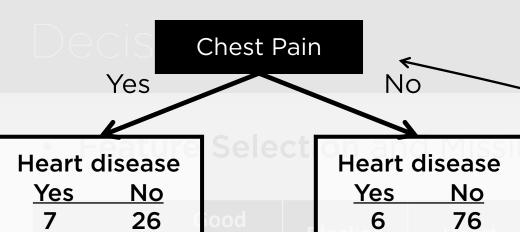


Chest pain	Good blood circulation	Blocked arteries	Heart disease	Good	d Circ.
No	No	No	No	Blocked	100/33
Yes	Yes	Yes	Yes		
Yes	Yes	No	No (	Chst Pn 13/102	92/3
Yes	No	?	Yes	17/3 7/22	8/0



Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	?	Yes



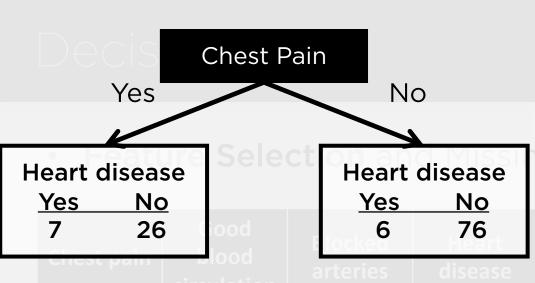


Gini impurity for Chest Pain = 0.29

6

7

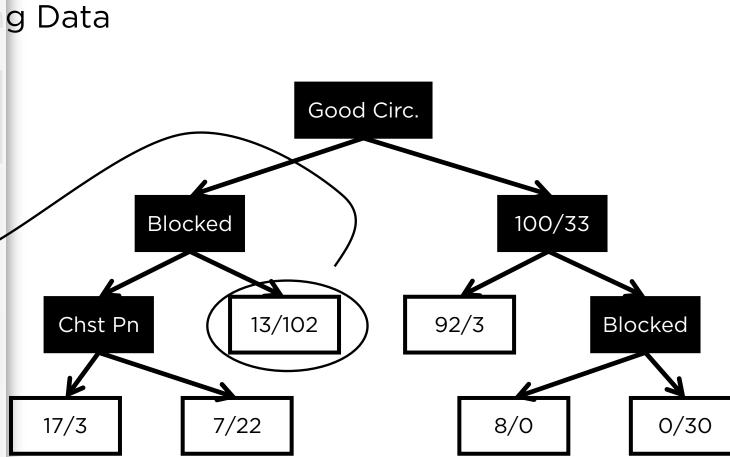
Data g Good Circ. 100/33 Blocked 13/102 Chst Pn 92/3 Blocked 8/0 0/30 17/3 7/22



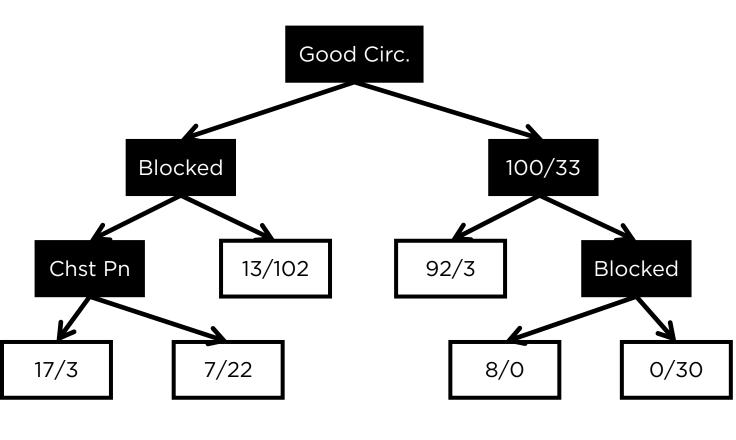
 $Gini\ impurity for\ Chest\ Pain=0.29$ 

Heart disease
Yes No
13 02

Gini impurity for Chest Pain = (0.20)



Chest pain	Good blood circulation	Blocked arteries	Heart disease
No	No	No	No
Yes	Yes	Yes	Yes
Yes	Yes	No	No
Yes	No	Ş	Yes

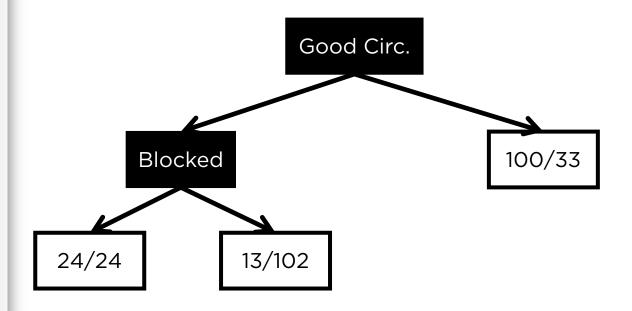


If Chest Pain does not reduce impurity score,

It would not be used to separate patients, and it would not be part of our tree.

Even though we have data for Chest Pain, it is no longer part of our tree.

Data



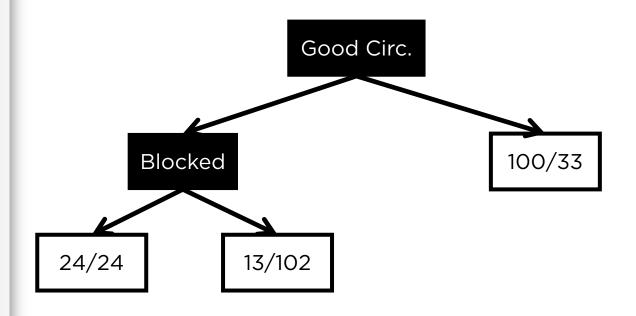
Automatic feature selection

Over fit: the tree does well the original data – the data used to build the tree – but does not do well with any other data set.

Decision Trees have the downside of often being over fit.

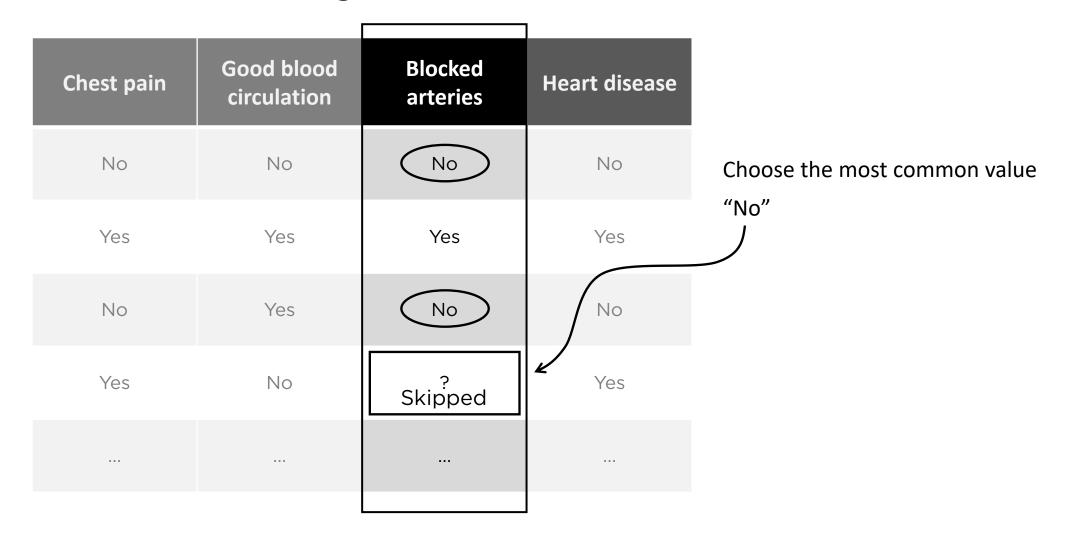
Need each split to make a large reduction in impurity.

) Data

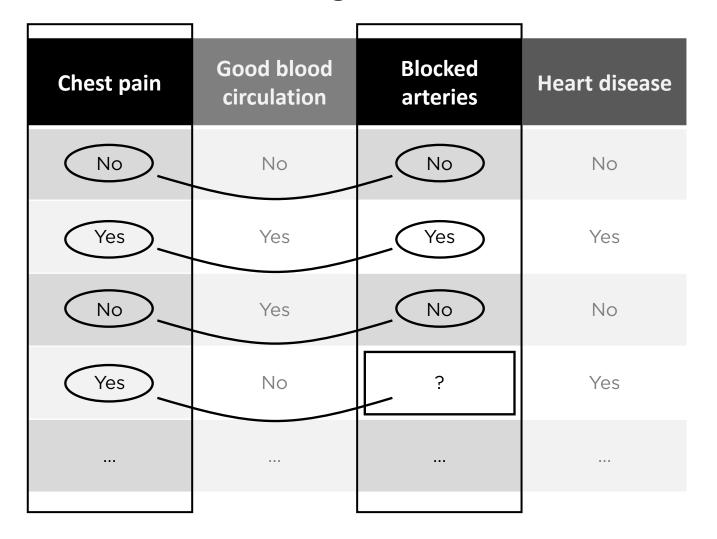


Automatic feature selection

- Not to "over fit"



Feature Selection and Missing Data



Find another column that has the highest correlation with blocked arteries and use that as a guide.

"Yes"

• Feature Selection and Missing Data

Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No
Yes	Yes	178	Yes
No	Yes	156	No
Yes	No	Ş	Yes

Weight data

- Mean / median

# Decision Trees

Feature Selection and Missing Data

Height	Good blood circulation	Weight	Heart disease
170cm	No	162	No
182cm	Yes	178	Yes
168cm	Yes	156	No
176cm	No	?	Yes

Find another column that has the highest correlation with weight and use that as a guide.

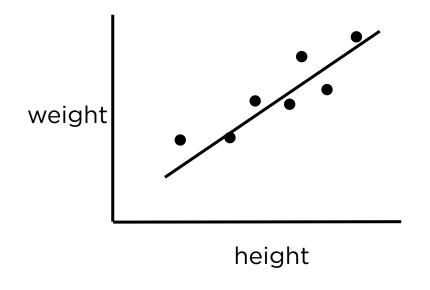
# Decision Trees

#### Feature Selection and Missing Data

Height	Good blood circulation	Weight	Heart disease
170cm	No	162	No
182cm	Yes	198	Yes
168cm	Yes	156	No
176cm	No	,	Yes

Find another column that has the highest correlation with weight and use that as a guide.

Do a linear regression on the two columns

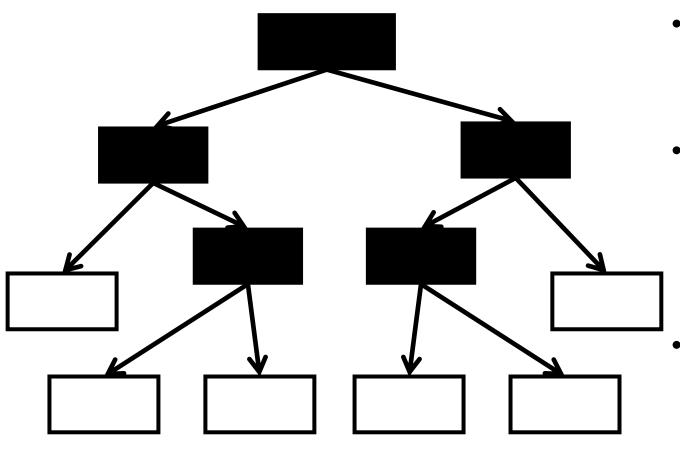


# Decision Trees

• Feature Selection and Missing Data

Height	Good blood circulation	Weight	Heart disease	Find another column that has the highest correlation with weight and use that as a guide.
170cm	No	162	No	Do a linear regression on the two columns  Use least squares line to predict the weight value
182cm	Yes	198	Yes	
168cm	Yes	156	No	
176cm	No	180	← Yes	weight
		i:		height

#### Why Random Forests



- Decision Trees are easy to build, use and interpret, but...
- Decision Trees are not flexible when classifying new samples.
  - -> accuracy not so good.
  - Random Forests combine the simplicity of Decision Trees with flexibility -> better accuracy.

How to build a Random Forest?

Step 1. Create a "bootstrapped" dataset.

#### **Original Dataset**

Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No
Yes	Yes	178	Yes
Yes	Yes	156	No
Yes	No	180	Yes

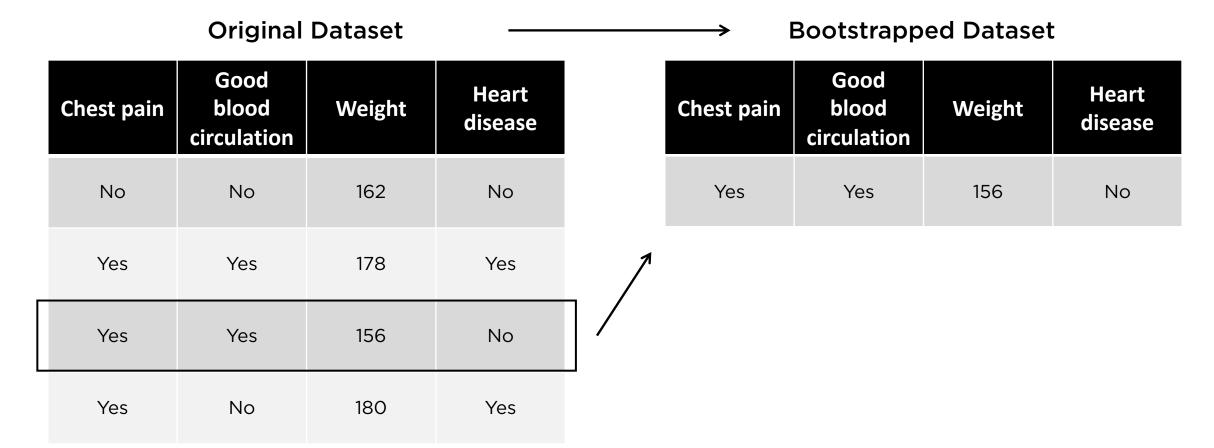
#### **Bootstrapped Dataset**

Chest pain blo	od	Weight	Heart disease
----------------	----	--------	------------------

- Same size as the original dataset.
- Randomly selected samples from the original dataset.
- Samples can be selected more than once.

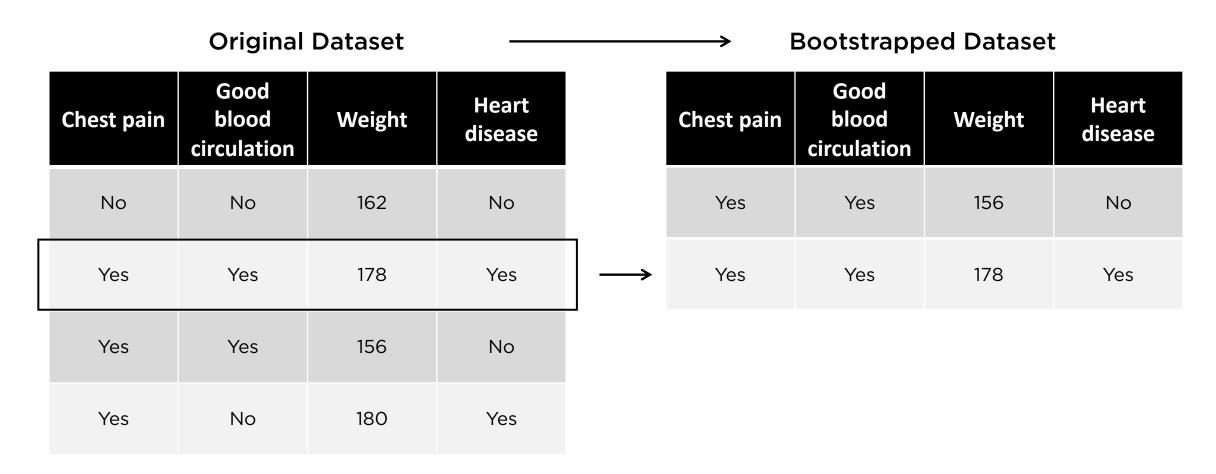
How to build a Random Forest?

Step 1. Create a "bootstrapped" dataset.



How to build a Random Forest?

Step 1. Create a "bootstrapped" dataset.



How to build a Random Forest?

Step 1. Create a "bootstrapped" dataset.

Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No
Yes	Yes	178	Yes
Yes	Yes	156	No
Yes	No	180	Yes

Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	156	No
Yes	Yes	178	Yes
Yes	No	180	Yes

How to build a Random Forest?

Step 1. Create a "bootstrapped" dataset.

**Original Dataset** 

**Bootstrapped Dataset** 

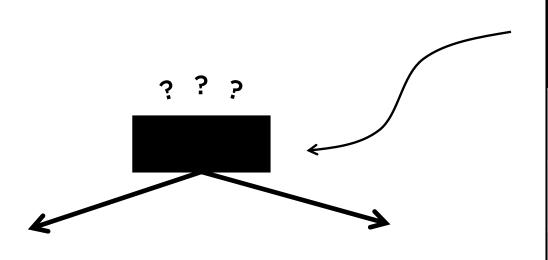
Chest pain	Good blood circulation	Weight	Heart disease	
No	No	162	No	
Yes	Yes	178	Yes	
Yes	Yes	156	No	_
Yes	No	180	Yes	

Chest pain	Good blood circulation	Weight	Heart disease	
Yes	Yes	156	No	
Yes	Yes	178	Yes	
Yes	No	180	Yes	7
Yes	No	180	Yes	m∈ ¥

How to build a Random Forest?

Step 2. Build a Decision Tree using the "bootstrapped" dataset, but only use a random subset of variables, e.g. 2

Bootstrapped Dataset

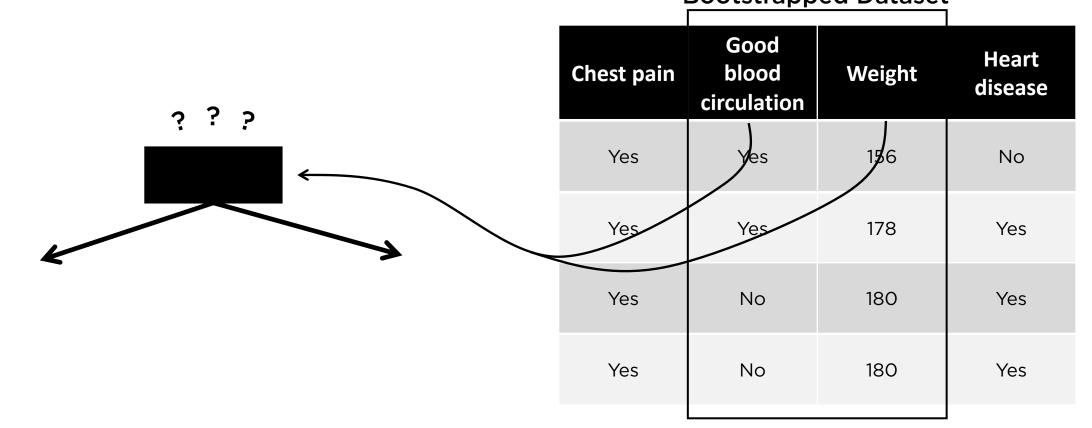


Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	156	No
Yes	Yes	178	Yes
Yes	No	180	Yes
Yes	No	180	Yes

How to build a Random Forest?

Step 2. Build a Decision Tree using the "bootstrapped" dataset, but only use a random subset of variables, e.g. 2

Bootstrapped Dataset

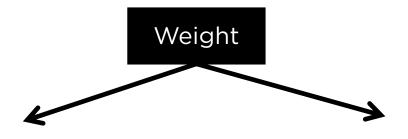


How to build a Random Forest?

Step 2. Build a Decision Tree using the "bootstrapped" dataset, but only use a random subset of variables, e.g. 2

Bootstrapped Dataset

Weight did the best job separating the samples.

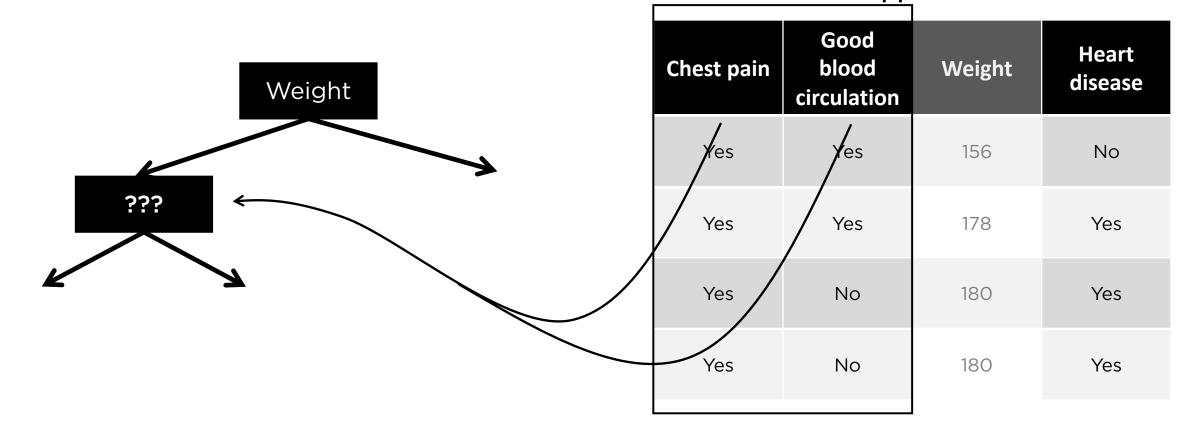


Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	156	No
Yes	Yes	178	Yes
Yes	No	180	Yes
Yes	No	180	Yes

How to build a Random Forest?

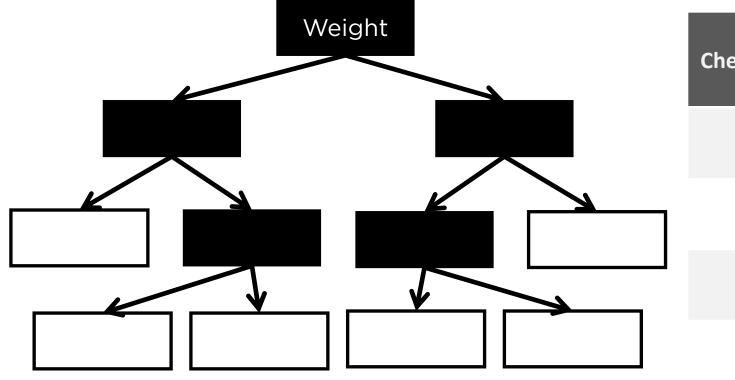
Step 2. Build a Decision Tree using the "bootstrapped" dataset, but only use a random subset of variables, e.g. 2

Bootstrapped Dataset



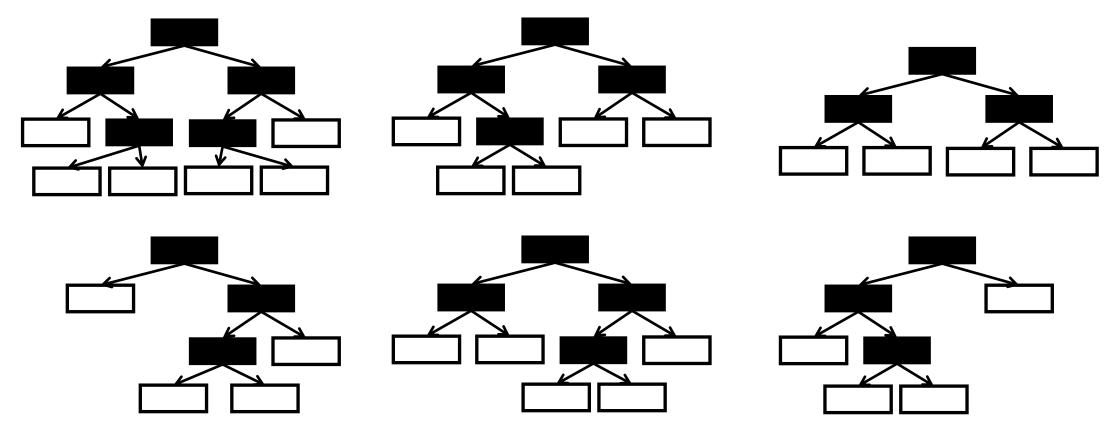
Step 2. Build a Decision Tree using the "bootstrapped" dataset, but only use a random subset of variables, e.g. 2

Bootstrapped Dataset

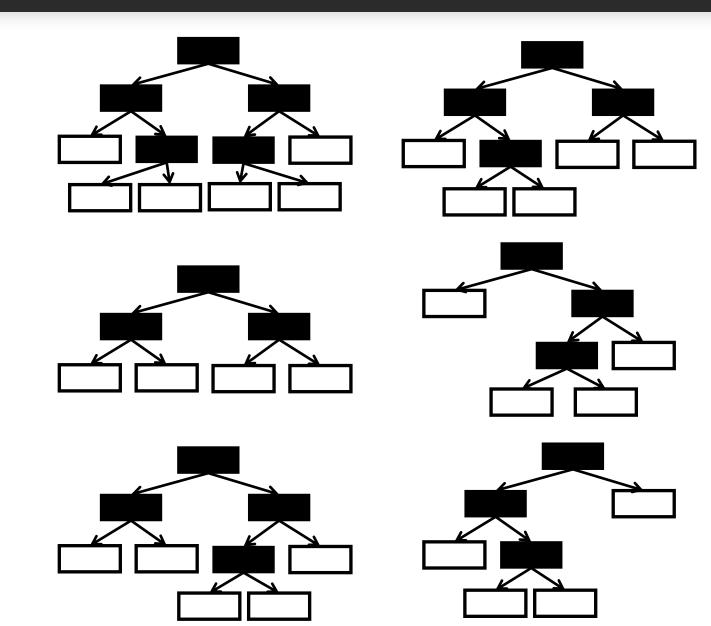


Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	156	No
Yes	Yes	178	Yes
Yes	No	180	Yes
Yes	No	180	Yes

Step 3. Go back to Step 1 and repeat: make a new bootstrap dataset and build a tree considering a subset of variables at each step. (ideally 100's of times )



- Using a bootstrapped sample and considering only a subset of the variables at each step results in a wide variety of trees.
- The variety makes Random
   Forests more effective than individual Decision Trees.



How to use a Random Forest?

How to use a Random Forest?

Get a new patient.

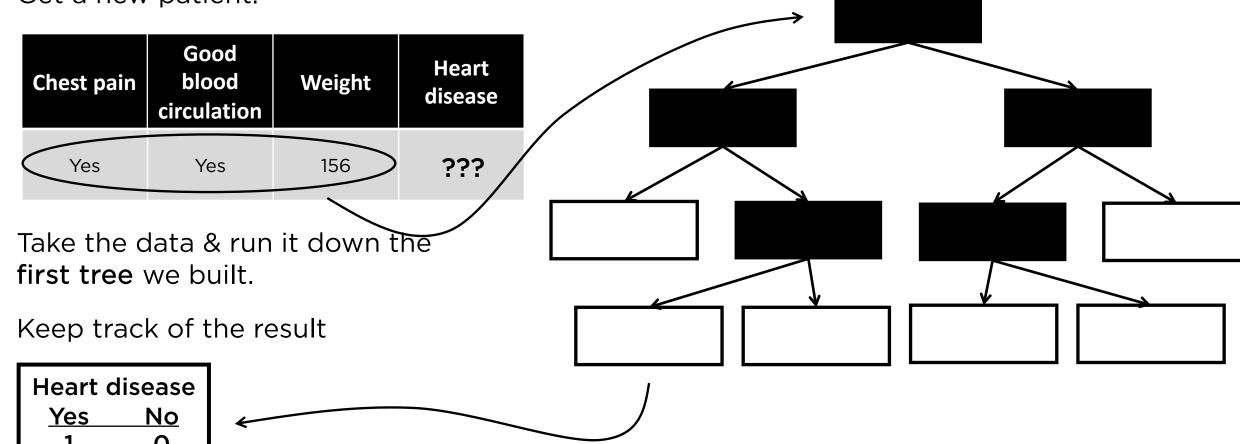
Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	156	???

With all the measurements.

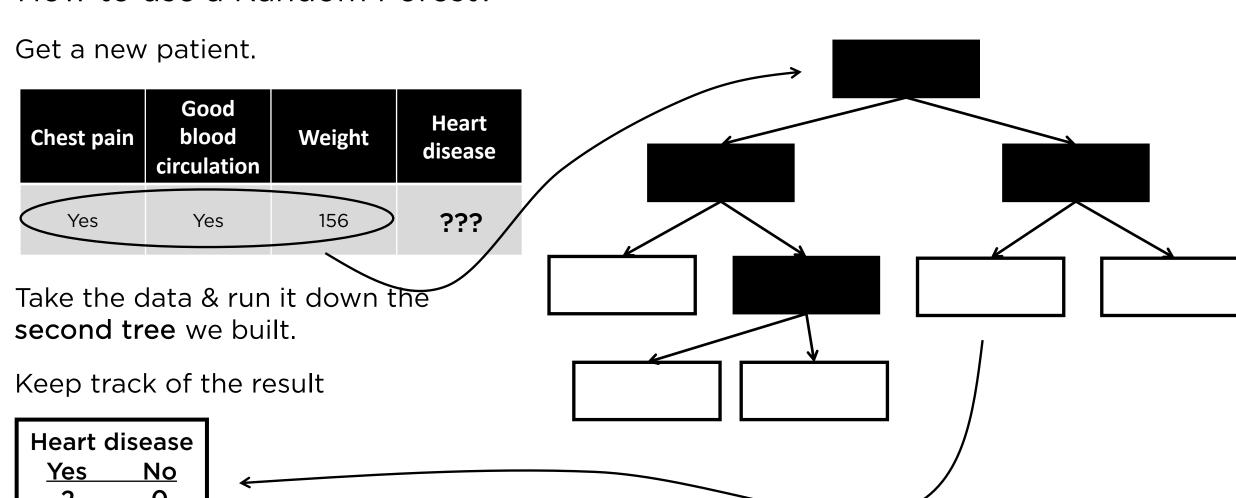
If the patient have heart disease?

How to use a Random Forest?





How to use a Random Forest?



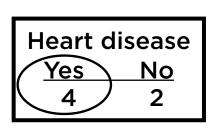
How to use a Random Forest?

Get a new patient.



Take the data & run it down the all the trees we built.

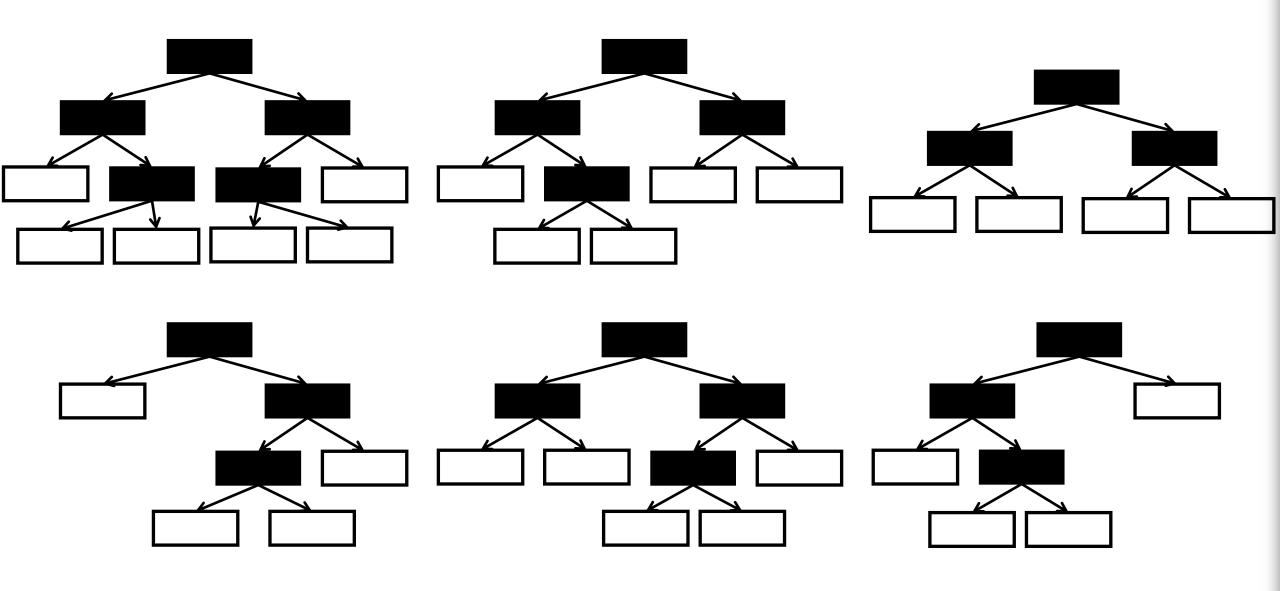
Which option received more votes.



#### **Terminology**

Bootstrapping the data plus using the aggregate to make a decision is called Bagging.





Is this Random Forest any good?

#### Typically,

About 1/3 of the original data does NOT end up in the bootstrapped dataset.

lood?

rt

ase

#### **Bootstrapped Dataset**

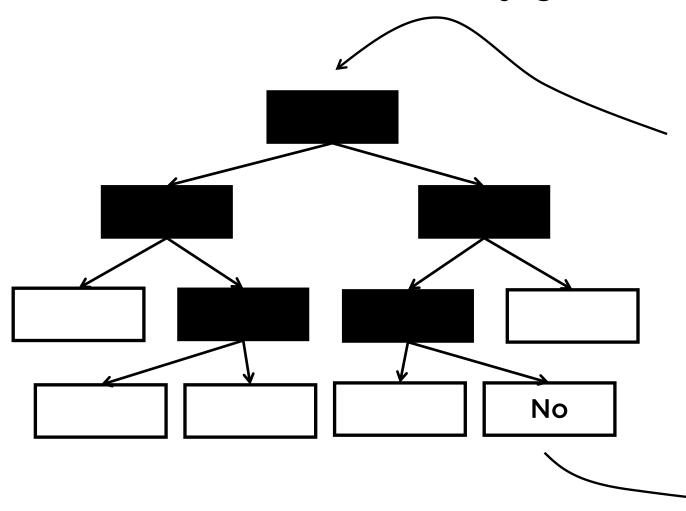
Good Heart **Chest pain** Weight blood disease circulation Yes Yes 156 No Yes Yes 178 Yes Yes Yes No 180 Yes No 180 Yes

**Duplicate entries** 

#### Is this Random Forest any good?

#### **Original Dataset** "Out-Of-Bag" Dataset Good Good Heart Heart **Chest pain** Weight **Chest pain** blood blood Weight disease disease circulation circulation No No No 162 No No No 162 Not included Yes Yes 178 Yes Entries Not in the Bootstrapped Dataset There would be more entry, if the Yes Yes 156 No original dataset were larger. Yes No 180 Yes

Is this Random Forest any good?

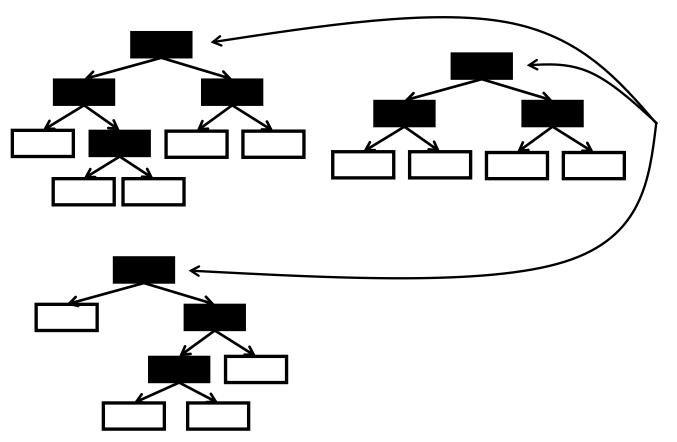


"Out-Of-Bag" Dataset

Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No

Run the data through and see if it correctly classifies the sample as "No Heart Disease"

Is this Random Forest any good?

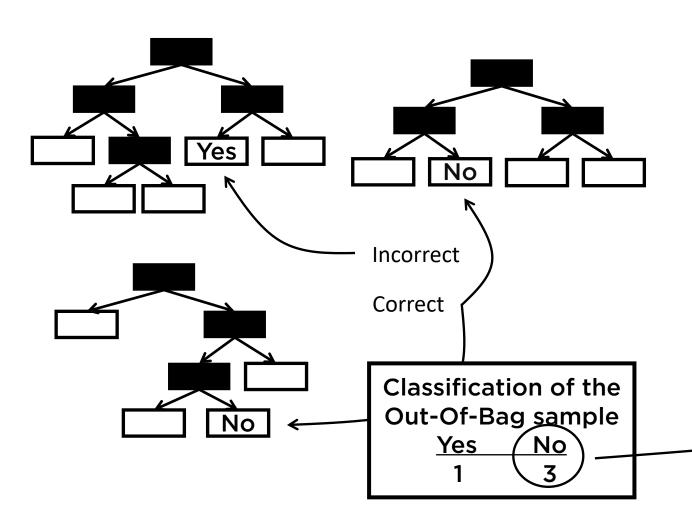


"Out-Of-Bag" Dataset

Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No

Then, run this Out-Of-Bag sample through all of the other trees that were built without it.

Is this Random Forest any good?



"Out-Of-Bag" Dataset

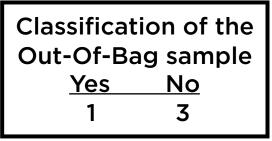
Chest pain	Good blood circulation	Weight	Heart disease
No	No	162	No

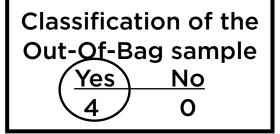
Then, run this Out-Of-Bag sample through all of the other trees that were built without it.

This sample is correctly labeled by the Random Forest.

#### Is this Random Forest any good?

Correct





"Out-Of-Bag" Dataset

Chest pain	Good blood circulation	Weight	Heart disease
Yes	No	156	Yes

Then, do the same thing for all of the other Out-Of-Bag samples for all of the trees.

#### Is this Random Forest any good?

Classification of the Out-Of-Bag sample

Yes No

1 3

Classification of the Out-Of-Bag sample

Yes No
4 0

Classification of the Out-Of-Bag sample

Yes No
1 3

Etc. ...

Incorrect

#### "Out-Of-Bag" Dataset

Chest pain	Good blood circulation	Weight	Heart disease
Yes	Yes	176	Yes

Then, do the same thing for all of the other Out-Of-Bag samples for all of the trees.

#### Is this Random Forest any good?

Classification of the Out-Of-Bag sample

Yes No
1 3

Classification of the Out-Of-Bag sample

Yes No
4 0

Classification of the Out-Of-Bag sample
Yes No
1 3

- Measure accuracy our Random Forest is by the proportion of Out-Of-Bag samples that were correctly classified by the Random Forest.
- The proportion of Out-Of-Bag samples that were incorrectly classified is the "Out-Of-Bag Error"

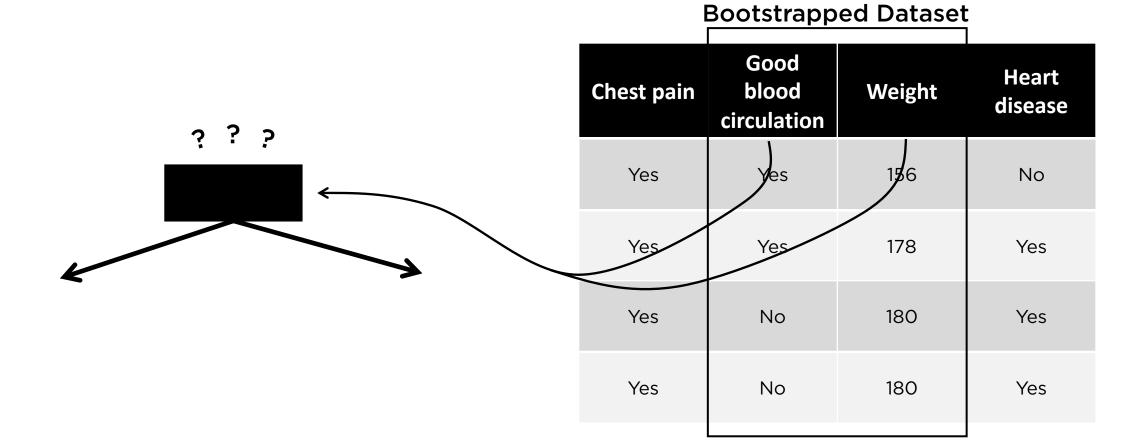
Now we know how to:

1. Build a Random Forest

2. Use a Random Forest

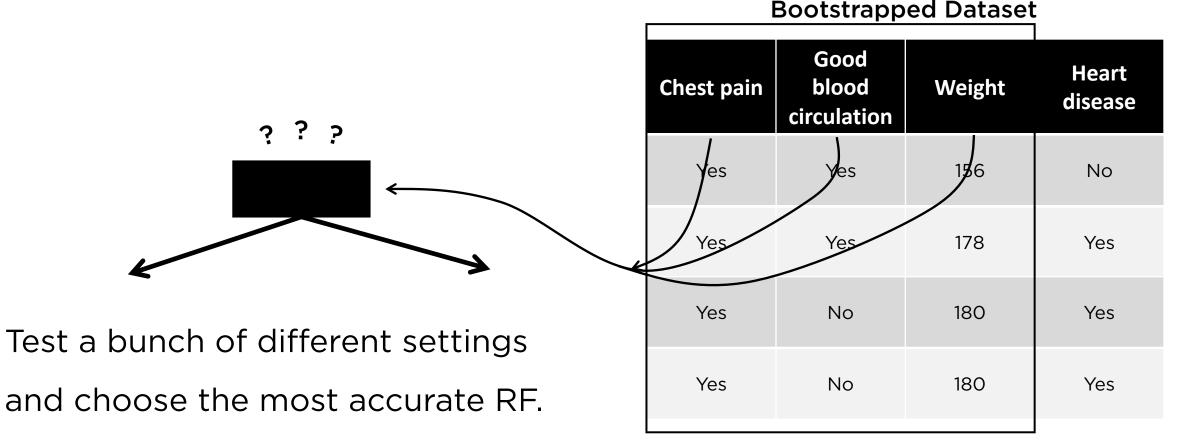
3. Estimate the Accuracy of a Random Forest

When we built our first tree and we only used two variables to make a decision at each step.



Compare Random Forest built using 2 variables per step...

... to Random Forest built using 3 variables per step.



So...

1. Build a Random Forest

Change the number of variables used per step

2. Estimate the Accuracy of a Random Forest

- Do this for a bunch of times and then choose the one that is most accurate.
- Typically, we start by using the square of the number of variables and then try
  a few settings above and below that value.