StatQuest: Random Forests Part 2, Missing data and sample clustering

Missing Data Filling

Original Dataset

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	???	???) No

Random Forests consider 2 types of missing data...

Original Dataset

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	???	???	No

- 1) Missing data in the original dataset used to create the random forest.
- 2) Missing data in a new sample that you want to categorize.

New Sample

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	???	

So we want to create a random forest from this data...

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No



However, we don't know if this patient has blocked arteries or their weight.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

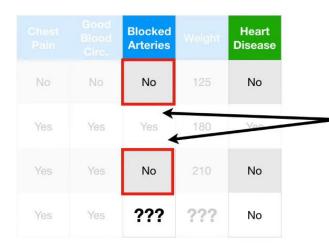
The general idea for dealing with missing data in this context is to make an initial guess that could be bad, then gradually refine the guess until it is (hopefully) a good guess.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

Because this person *did not* have **Heart Disease**...

		Blocked Arteries		Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

...the initial, and possibly bad, guess for the blocked arteries value is just the most common value for "Blocked Arteries" found in the other samples that **do not** have Heart Disease.



Among the people that do not have Heart Disease, "No" is the most common value for Blocked arteries - it occurs in 2 out of 2 samples.

		Blocked Arteries		Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	(No	???	No

So "No" is our initial guess.



Since **weight** is numeric, our initial guess will be the median value of the patients that *did not* have heart disease.

				Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Here's our new dataset with the filled in missing values...

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Now we want to refine these guesses.

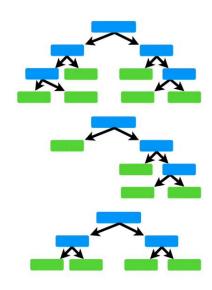
We do this by first determining which samples are similar to the one with missing data.

So let's talk about how to determine similarity...

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

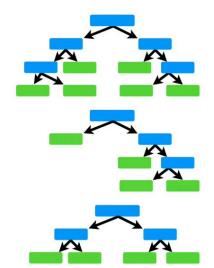
Step 1: Build a random forest...



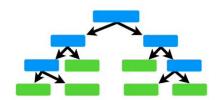
Step 2: Run all of the data down all of the trees.

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No



Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No



We'll start by running all of the data down the first tree.



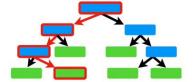




Notice that Sample 3 and Sample 4 both ended up at the same leaf node.

Filled-in Missing Values





That means they are similar.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

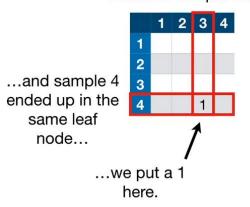
We keep track of similar samples using a "Proximity Matrix"

	1	2	3	4
1				
2				
3				
4				

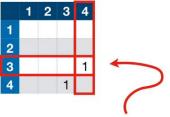
Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Because sample 3...



Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No



We also put a 1 here, since this position also represents samples 3 and 4.

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Because no other pair of samples ended in the same leaf node, our proximity matrix looks like this after running the samples down the first tree.

	1	2	3	4
1				
2				
3				1
4			1	

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

Ultimately, we run the data down all the trees and the proximity matrix fills in.

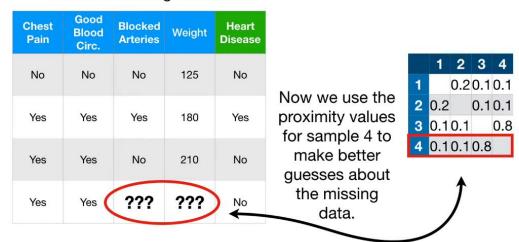
	1	2	3	4
1		2	1	1
2	2		1	1
3	1	1		8
4	1	1	8	

Filled-in Missing Values

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	No	167.5	No

1 2 3 4 1 0.2 0.1 0.1 2 0.2 0.1 0.1 3 0.1 0.1 0.8 4 0.1 0.1 0.8

Then we divide each proximity value by the total number of trees. In this example, assume we had 10 trees.



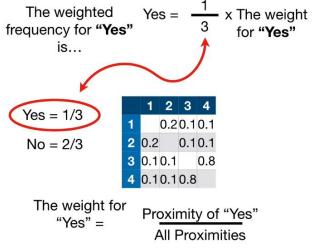
Filled-in Missing Values

		Blocked Arteries		
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

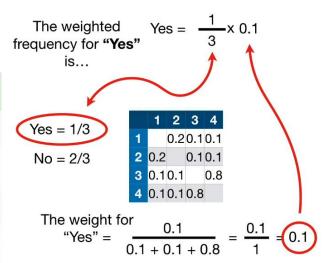
For Blocked Arteries, we calculate the weighted frequency of "Yes" and "No, using proximity values as the weights.







		Blocked Arteries		
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No



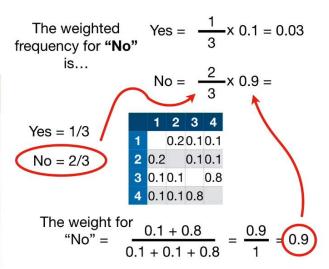
Filled-in Missing Values

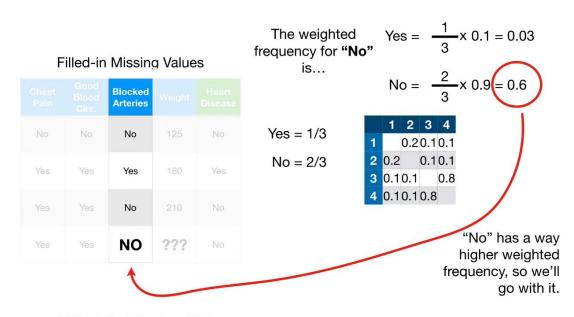
		Blocked Arteries		
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

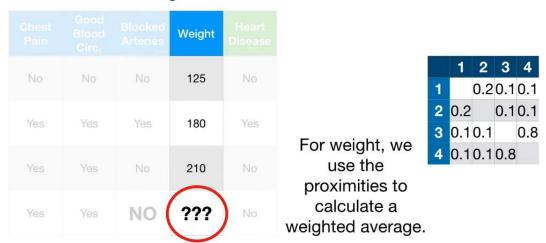
The weighted frequency for "Yes" Yes =
$$\frac{1}{3}$$
x 0.1 = 0.03

The weighted frequency for "Yes".

		Blocked Arteries		
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	???	???	No

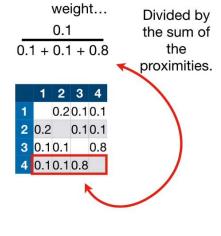


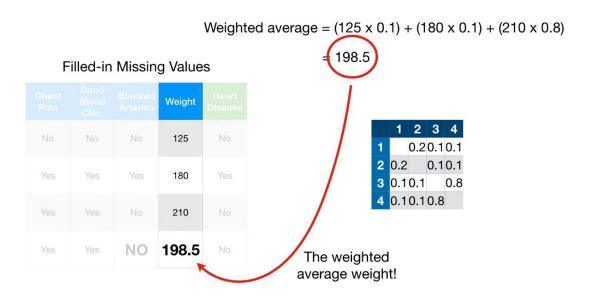






			Weight	
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	NO	???	No





Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	Yes	NO	198.5	No

Now that we've revised our guesses a little bit, we do the whole thing over again...

We build a random forest, run the data through the trees, recalculate the proximities and recalculate the missing values.

We do this 6 or 7 times until the missing values converge (i.e. no longer change each time we recalculate).

Random Forests consider 2 types of missing data...

1) Missing data in the original dataset used to create the random forest.

At long last, we'll talk about the second method!

Missing data in a new sample that you want to categorize.

New Sample

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	???	

Imagine we had already built a Random Forest with existing data and wanted to classify this new patient.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	\bigcirc

So we want to know if they have heart disease or not...

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	

...but we don't know if they have blocked arteries...

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	

...so we need to make a guess about Blocked Arteries so we can run the patient down all the trees in the forest.



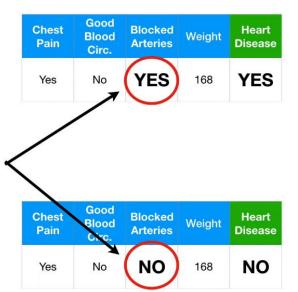
The first thing we do is create two copies of the data, one that has heart disease...

Ches Pain	Blood	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	NO

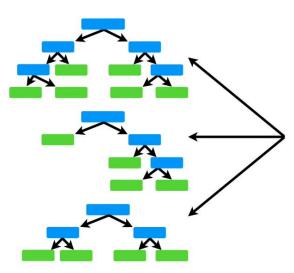
Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	YES

...and one that doesn't have heart disease.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	???	168	NO



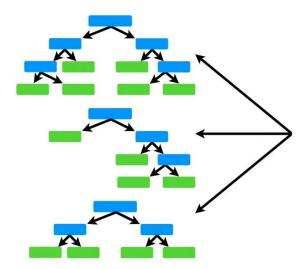
Then we use the iterative method we just talked about to make a good guess about the missing values.



Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	(YES)	168	YES

Then we run the two samples down the trees in the forest...

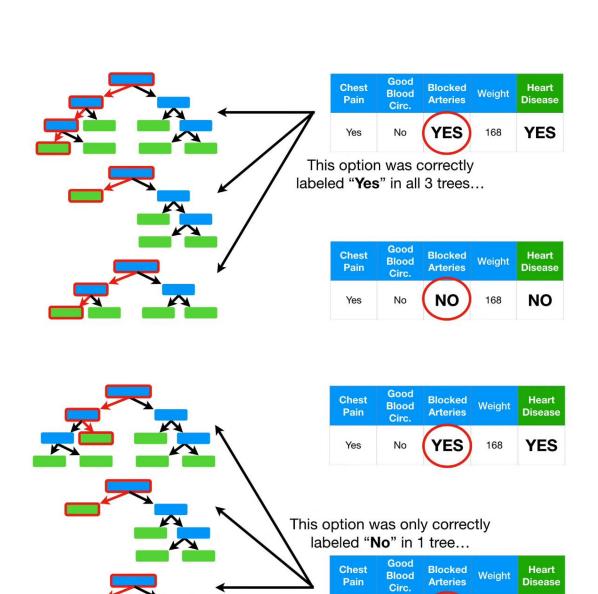
Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	(NO)	168	NO

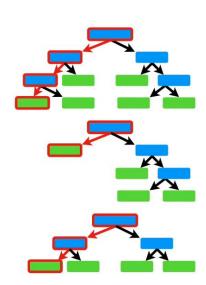


Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	YES	168	YES

...and we see which of the two is correctly labeled by the random forest the most times.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	(NO)	168	NO





	Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
1	Yes	No	YES	168	YES

NO

NO

Yes

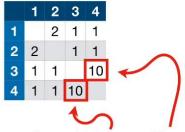
No

This option wins because it was correctly labeled more than the other option.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	NO	168	NO

Sample Clustering

Just for the sake of easy math, imagine if Samples 3 and 4 ended up in the same leaf node in all 10 trees.



Now we have 10 here and here...

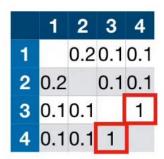
After dividing by 10 (the number of trees in the forest), we see that the largest number in the proximity matrix is 1.

	1	2	3	4
1		2	1	1
2	2		1	1
3	1	1		10
4	1	1	10	

	1	2	3	4
1		0.2	0.1	0.1
2	0.2		0.1	0.1
3	0.1	0.1		1
4	0.1	0.1	1	

1 in the proximity matrix means the samples are as close as close can be.





1 2 3 4 1 2 1 1 2 2 1 1 3 1 1 10 4 1 1 10



1 - the proximity values
= distance

1 2 3 4
1 0.80.90.9

0.90.9

2 0.8

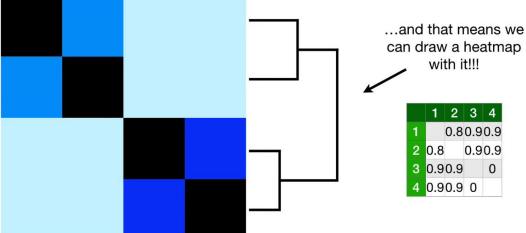
3 0.90.9

4 0.90.9 0

That means...

Sample 1 Sample 2 Sample 3 Sample 4

This is a distance matrix...



This is a distance matrix...

