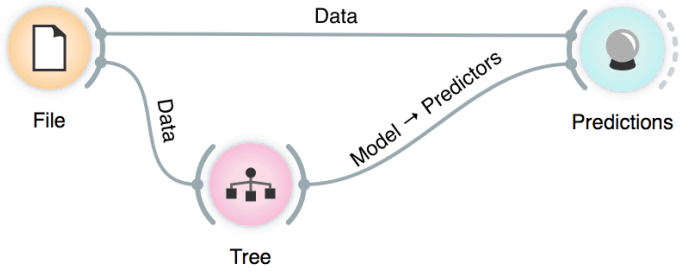
Lesson 5: Classification

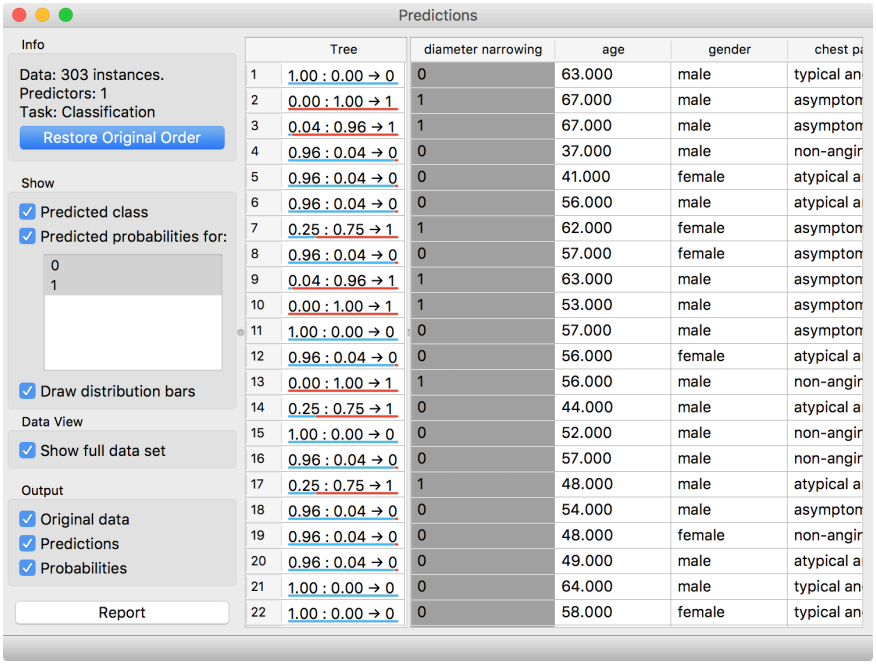
In one of the previous lessons, we explored the heart disease data. We wanted to predict which persons have clogged arteries — but we did not make any predictions. We observed some potentially interesting relations between the features and the condition, but we never constructed an actual model.

Let us create one now.



We call the variable we wish to predict a target variable, or an outcome or, in traditional machine learning terminology, a class. Hence we talk about classification, classifiers, classification trees...

The data is fed into the Tree widget, which uses it to infer a predictive model. The Predictions widget gets the data from the File widget and a predictive model from the Tree widget. This is something new: in our past workflows, widgets passed only data to each other, but here we have a channel that carries a model.



	Tree	diameter narrowing	age	gender	chest pa
1	1.00 : 0.00 → 0	0	63.000	male	typical an
2	0.00 : 1.00 → 1	1	67.000	male	asympton
3	0.04 : 0.96 → 1	1	67.000	male	asympton
4	0.96 : 0.04 → 0	0	37.000	male	non-angir
5	0.96 : 0.04 → 0	0	41.000	female	atypical a
6	0.96 : 0.04 → 0	0	56.000	male	atypical a
7	0.25 : 0.75 → 1	1	62.000	female	asympton
8	0.96 : 0.04 → 0	0	57.000	female	asympton
9	0.04 : 0.96 → 1	1	63.000	male	asympton
10	0.00 : 1.00 → 1	1	53.000	male	asympton
11	1.00 : 0.00 → 0	0	57.000	male	asympton
12	0.96 : 0.04 → 0	0	56.000	female	atypical a
13	0.00 : 1.00 → 1	1	56.000	male	non-angir
14	0.25 : 0.75 → 1	0	44.000	male	atypical a
15	1.00 : 0.00 → 0	0	52.000	male	non-angir
16	0.96 : 0.04 → 0	0	57.000	male	non-angir
17	0.25 : 0.75 → 1	1	48.000	male	atypical a
18	0.96 : 0.04 → 0	0	54.000	male	asympton
19	0.96 : 0.04 → 0	0	48.000	female	non-angir
20	0.96 : 0.04 → 0	0	49.000	male	atypical a
21	1.00 : 0.00 → 0	0	64.000	male	typical an
22	1.00 : 0.00 → 0	0	58.000	female	typical an

The Predictions widget uses the model to make predictions about the data and shows them in the table.

How correct are these predictions? Do we have a good model? How can we tell?

But (and even before answering these critical questions), what is a tree? How does it look like? How does Orange create one? Is this algorithm something we should use?

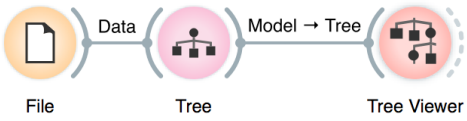
So many questions to answer today!

Lesson 6: Classification Trees

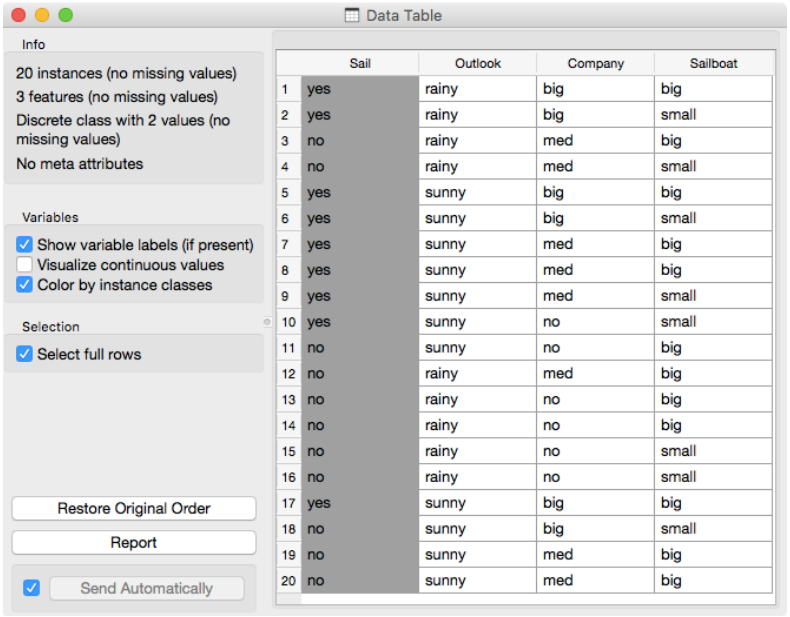
Classification tree is one of the oldest, but still popular, machine learning methods. We like it since the method is easy to explain and gives rise to random forests, one of the most accurate machine learning techniques (more on this later). So, what kind of model is a classification tree?

Let us load a data set from http://file.biolab.si/datasets/sailing.tab that records the conditions under which a friend skipper went sailing, build a tree and visualize it in the Tree Viewer.

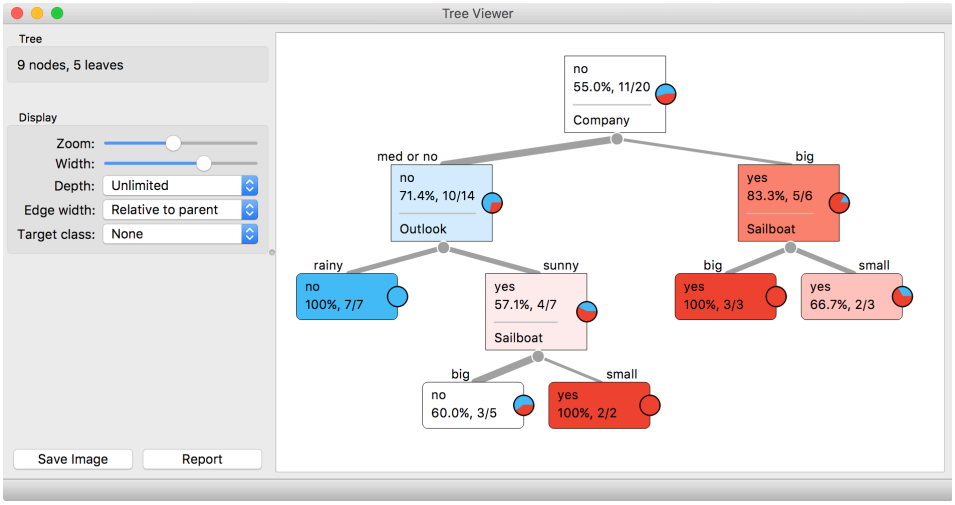
The data set we will use is stored on a server. Copy the web address and paste it into URL entry box in the File widget. An alternative way to access this data is to use the Data Sets widget that is currently available in the Prototypes add-on.



Here's a warning: this sailing data is small. Therefore, any relations inferred from the classification tree on this page are unreliable. What should the size of the data set be to acquire stronger conclusions?



	Sail	Outlook	Company	Sailboat
1	yes	rainy	big	big
2	yes	rainy	big	small
3	no	rainy	med	big
4	no	rainy	med	small
5	yes	sunny	big	big
6	yes	sunny	big	small
7	yes	sunny	med	big
8	yes	sunny	med	big
9	yes	sunny	med	small
10	yes	sunny	no	small
11	no	sunny	no	big
12	no	rainy	med	big
13	no	rainy	no	big
14	no	rainy	no	big
15	no	rainy	no	small
16	no	rainy	no	small
17	yes	sunny	big	big
18	no	sunny	big	small
19	no	sunny	med	big
20	no	sunny	med	big



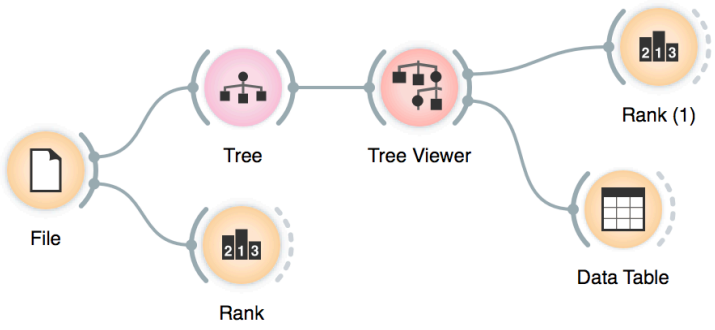
We read the tree from top to bottom. It looks like this skipper is a social person; as soon as there's company, the probability of her sailing increases. When joined by a smaller group of individuals, there is no sailing if there is rain. (Thunderstorms? Too dangerous?) When she has a smaller company, but the boat at her disposal is big, there is no sailing either.

Classification trees were hugely popular in the early years of machine learning, when they were first independently proposed by the engineer Ross Quinlan (C4.5) and a group of statisticians (CART), including the father of random forests Leo Brieman.

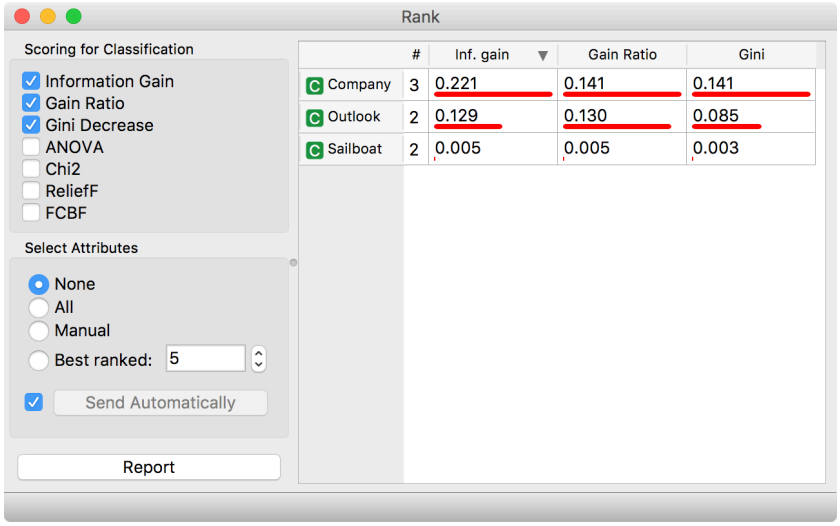
Trees place the most useful feature at the root. What would be the most useful feature? It is the feature that splits the data into two purest possible subsets. These are then split further, again by the most informative features. This process of breaking up the data subsets to smaller ones repeats until we reach subsets where all data belongs to the same class. These subsets are represented by leaf nodes in strong blue or red. The process of data splitting can also terminate when it runs out of data instances or out of useful features (the two leaf nodes in white).

The Rank widget could be used on its own. Say, to figure out which genes are best predictors of the phenotype in some gene

We still have not been very explicit about what we mean by "the most useful" feature. There are many ways to measure this. We can compute some such scores in Orange using the Rank widget, which estimates the quality of data features and ranks them according to how much information they carry. We can compute the scores from the whole data set or from data corresponding to some node of the classification tree in the Tree Viewer.



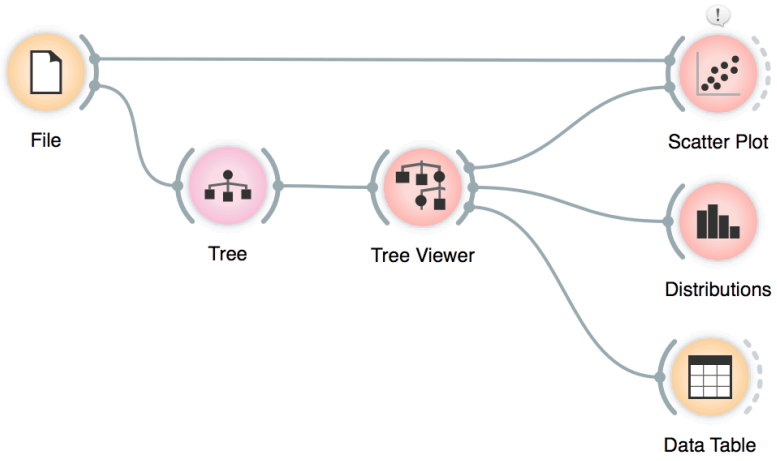
In this class, we will not dive into definitions. If you are interested, there's a good explanation of information gain on stackoverflow.com.



Lesson 7: Model Inspection

Here's another interesting combination of widgets: the classification tree viewer and the scatterplot. This time, consider the famous Iris data set (comes with Orange). In the Scatter Plot, find the best visualization of this data set, that is, the one that best separates the instances from different classes. Then connect the Tree Viewer to the Scatterplot. Selecting any node of the tree will output the corresponding data subset, which will be shown in the scatter plot.

Wherever possible, visualizations in Orange are designed to support selection and passing of the data that applies to it. Finding interesting data subsets and analyzing their commonalities is a central part of explorative data analysis, a data analysis approach favored by the data visualization guru Edward Tufte.

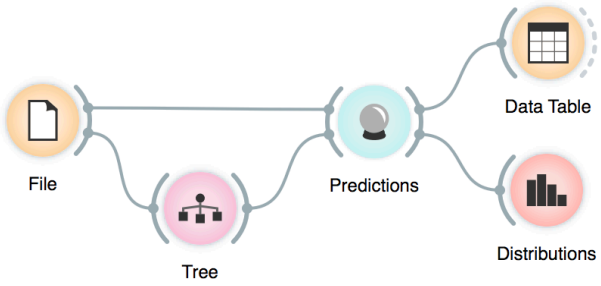


Just for fun, we have included a few other widgets in this workflow. In a way, the Tree Viewer widget behaves like the Select Rows widget, except that the rules used to filter the data are inferred from the data itself and optimized to obtain purer data subsets.

Lesson 8: Classification Accuracy

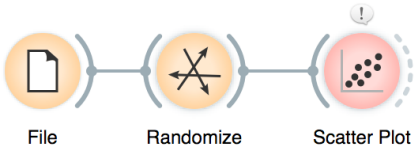
Now that we know what classification trees are, the next question is what is the quality of their predictions. For beginning, we need to define what we mean by quality. In classification, the simplest measure of quality is classification accuracy expressed as the proportion of data instances for which the classifier correctly guessed the value of the class. Let's see if we can estimate, or at least get a feeling for, classification accuracy with the widgets we already know.

Measuring of accuracy is such an important concept that it would require its widget. But wait a while, there's educational value in reusing the widgets we already know.



Let us try this schema with the brown-selected data set. The Predictions widget outputs a data table augmented with a column that includes predictions. In the Data Table widget, we can sort the data by any of these two columns, and manually select data instances where the values of these two features are different (this would not work on big data). Roughly, visually estimating the accuracy of predictions is straightforward in the Distribution widget, if we set the features in view appropriately.

This lesson has a strange title and it is not obvious why it was chosen. Maybe you, the reader, should tell us what does this lesson have to do with cheating.

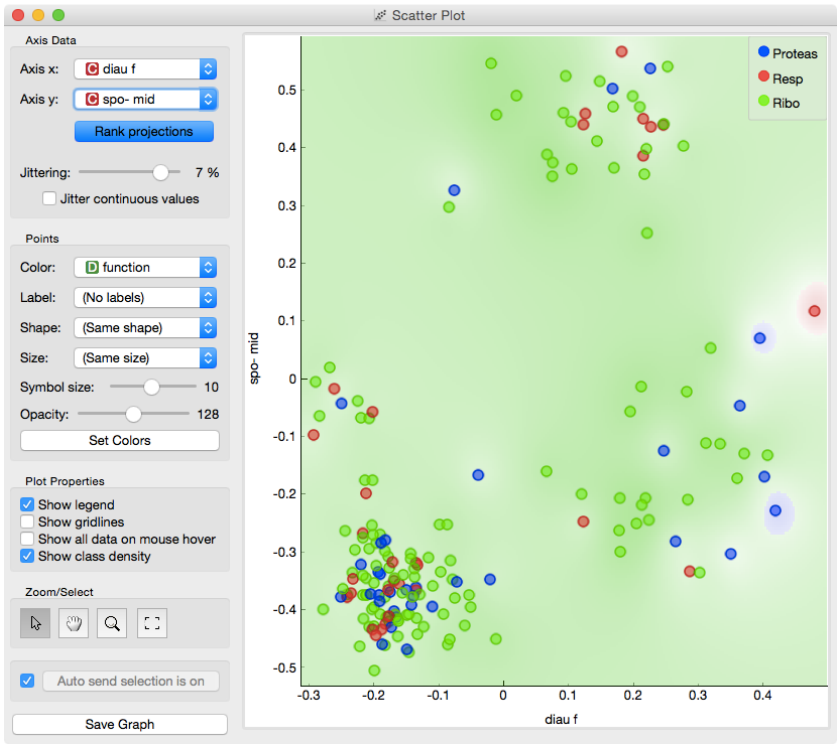


Randomize widget shuffles the column in the data table. It can shuffle the class column, columns with data features or columns with meta information. Shuffling the class column breaks any relation between features and the class, keeping the data points (genes profiles) intact.

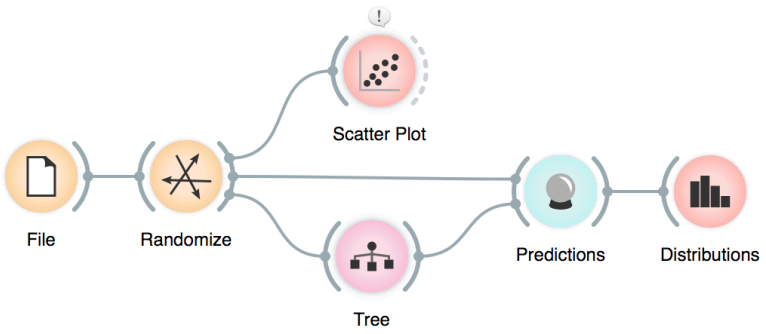
Why is the background in this scatter plot so green, and only green? Why have the other colors disappeared after the class randomization?

Lesson 9: How to Cheat

At this stage, the classification tree looks very good. There's only one data point where it makes a mistake. Can we mess up the data set so bad that the trees will ultimately fail? Like, remove any existing correlation between gene expression profiles and class? We can! There's the Randomize widget that can shuffle the class column. Check out the chaos it creates in the Scatter Plot visualization where there were nice clusters before randomization!

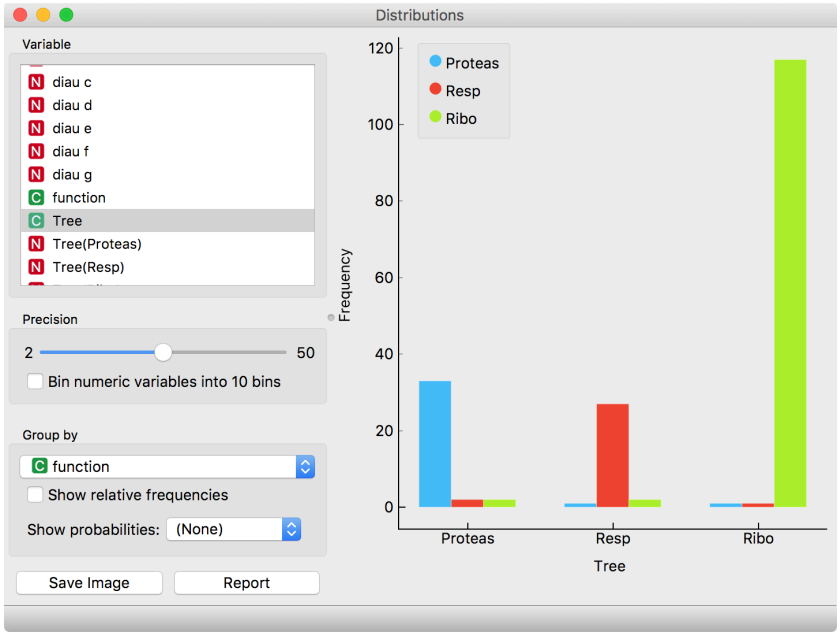


Fine. There can be no classifier that can model this mess, right? Let us test this. We will build classification tree and check its performance on the messed-up data set.



And the result? Here is a screenshot of the Distributions:

At this stage, it may be worthwhile checking how do the trees look. Try comparing the tree inferred from original and shuffled data!



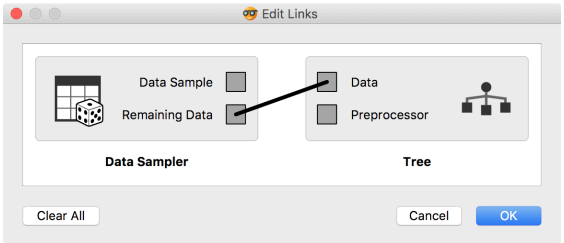
Most unusual. Almost no mistakes. How is this possible? On a class-randomized data set?

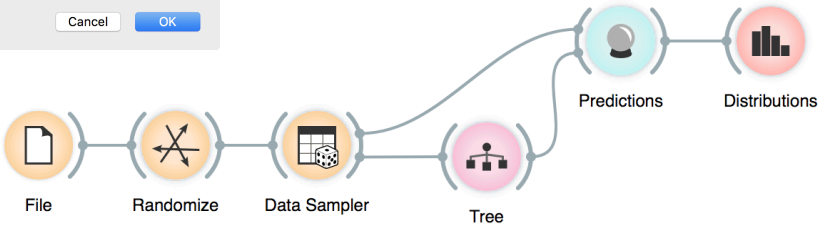
To find the answer to this riddle, open the Tree Viewer and check out the tree. How many nodes does it have? Are there many data instances in the leaf nodes?

It looks like the tree just memorized every data instance from the data set. No wonder the predictions were right. The tree makes no sense, and it is complex because it simply remembered everything.

Ha, if this is so, that is, if a classifier remembers everything from a data set but without discovering any general patterns, it should perform miserably on any new data set. Let us check this out. We will split our data set into two sets, training and testing, train the classification tree on the training data set and then estimate its accuracy on the test data set.

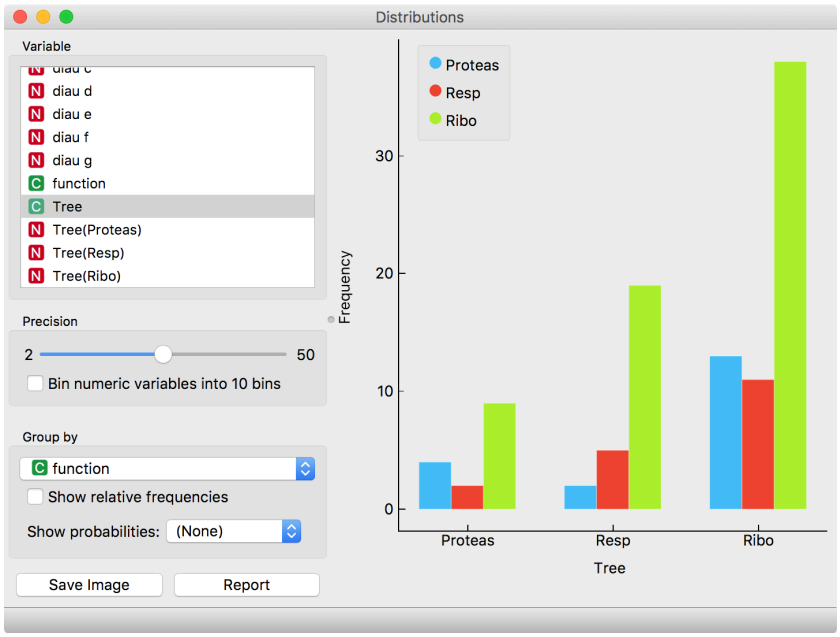
The signals from the Data Sampler widget have not been named in our workflow to save space. The Data Sampler splits the data to a sample and out-of-sample (so called remaining data). The sample was given to the Tree widget, while the remaining data was handed to the Predictions widget. Set the Data Sampler so that the size of these two data sets is about equal.





Let's check how the Distributions widget looks after testing the classifier on the test data.

Turns out that for every class value the majority of data instances has been predicted to the ribosomal class (green). Why? Green again (like green from the Scatter Plot of the messed-up data)? Here is a hint: use the Box Plot widget to answer this question.



The first two classes are a complete fail. The predictions for ribosomal genes are a bit better, but still with lots of mistakes. On the class-randomized training data, our classifier fails miserably. Finally, this is just as we would expect.

To test the performance (accuracy) of the classification technique, we have just learned that we need to train the classifiers on the training set and then test it on a separate test set. With this test, we can distinguish between those classifiers that just memorize the training data and those that learn a useful model.

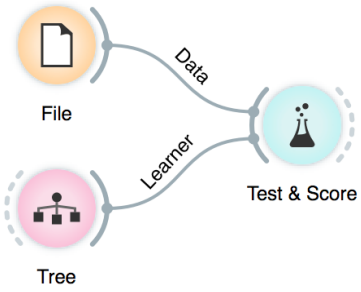
We needed to class-randomize only the training data set to fail in predictions. Try changing the workflow so that the classes are randomized only there, and not in the test set.

Learning is not only remembering. Rather, it is discovering patterns that govern the data and apply to new data as well. To estimate the accuracy of a classifier, we, therefore, need a separate test set. This assessment should not depend on just one division of the input data set to training and test set (here's a place for cheating as well). Instead, we need to repeat the process of estimation several times, each time on a different train/test set and report on the average score.

Lesson 10: Cross-Validation

Estimating the accuracy may depend on a particular split of the data set. To increase robustness, we can repeat the measurement several times, each time choosing a different subset of the data for training. One such method is cross-validation. It is available in Orange through the Test & Score widget.

Note that in each iteration, Test & Score will pick part of the data for training, learn the predictive model on this data using some machine learning method, and then test the accuracy of the resulting model on the remaining, test data set. For this, the widget will need on its input a data set from which it will sample data for training and testing, and a learning method which it will use on the training data set to construct a predictive model. In Orange, the learning method is simply called a learner. Hence, Test & Score needs a learner on its input. A typical workflow with this widget is as follows.



For geeks: a learner is an object that, given the data, outputs a classifier. Just what Test & Score needs.

This is another way to use the Tree widget. In the workflows from the previous lessons we have used another of its outputs, called Model: its construction required the data. This time, no data is needed for Tree, because all that we need from it a learner.

Here we show Test & Score widget looks like. CA stands for classification accuracy, and this is what we really care for for now. We will talk about other measures, like AUC, later.

Cross validation splits the data sets into, say, 10 different non-overlapping subsets we call folds. In each iteration, one fold will be used for testing, while the data from all other folds will be used for training. In this way, each data instance will be used for testing exactly once.