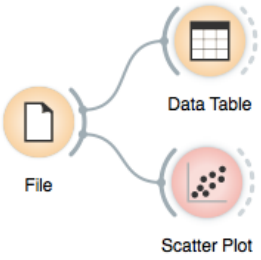
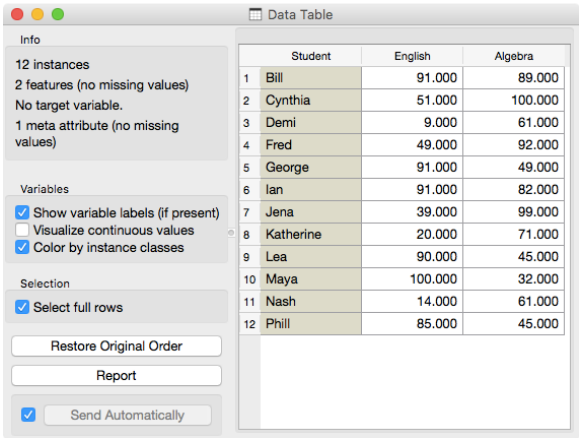
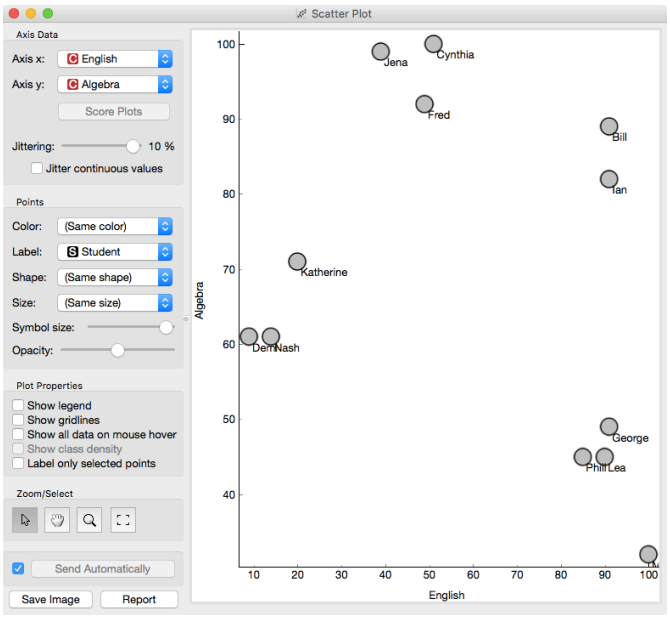
Lesson 26: Hierarchical Clustering

In the class, we will introduce clustering using a simple data set on students and their grades in English and Algebra. Load the data set from http://file.biolab.si/files/grades2.tab.

Say that we are interested in finding clusters in the data. That is, we would like to identify groups of data instances that are close together, similar to each other. Consider a simple, two-featured data set (see the side note) and plot it in the Scatter Plot. How many clusters do we have? What defines a cluster? Which data instances belong to the same cluster? What would a procedure for discovering clusters look like?







How do we measure the similarity between clusters if we only know the similarities between points? By default, Orange computes the average distance between all their pairs of data points; this is called average linkage. We could instead take the distance between the two closest points in each cluster (single linkage), or the two points that are furthest away (complete linkage).

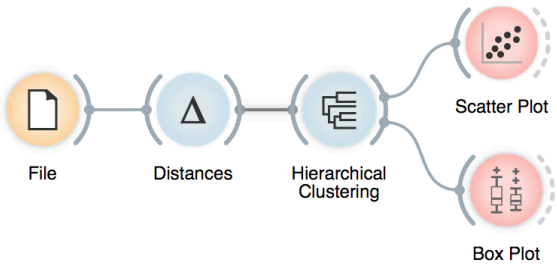
We need to start with a definition of "similar". One simple measure of similarity for such data is the Euclidean distance: square the differences across every dimension, some them and take the square root, just like in Pythagorean theorem. So, we would like to group data instances with small Euclidean distances.

Now we need to define a clustering algorithm. We will start with each data instance being in its own cluster. Next, we merge the clusters that are closest together - like the closest two points - into one cluster. Repeat. And repeat. And repeat. And repeat until you end up with a single cluster containing all points.

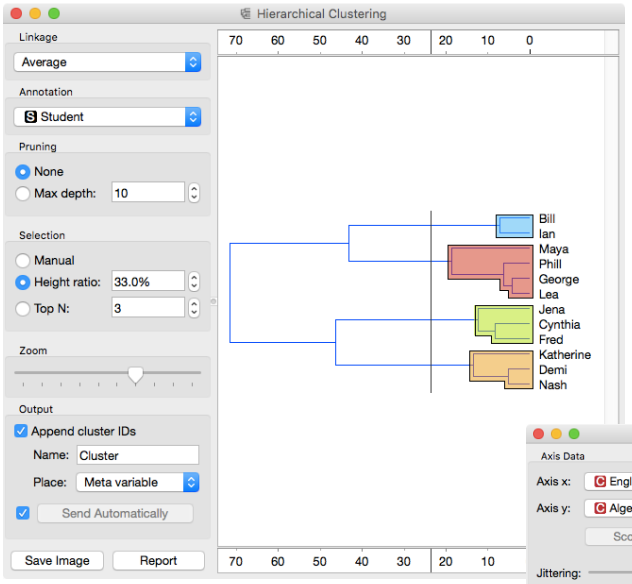
This procedure constructs a hierarchy of clusters, which explains why we call it hierarchical clustering. After it is done, we can

observe the entire hierarchy and decide which would be a good point to stop. With this we decide the actual number of clusters.

One possible way to observe the results of clustering on our small data set with grades is through the following workflow:



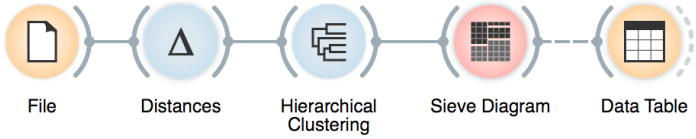
Let us see how this works. Load the data, compute the distances and cluster the data. In the Hierarchical clustering widget, cut hierarchy at a certain distance score and observe the corresponding clusters in the Scatter plot.



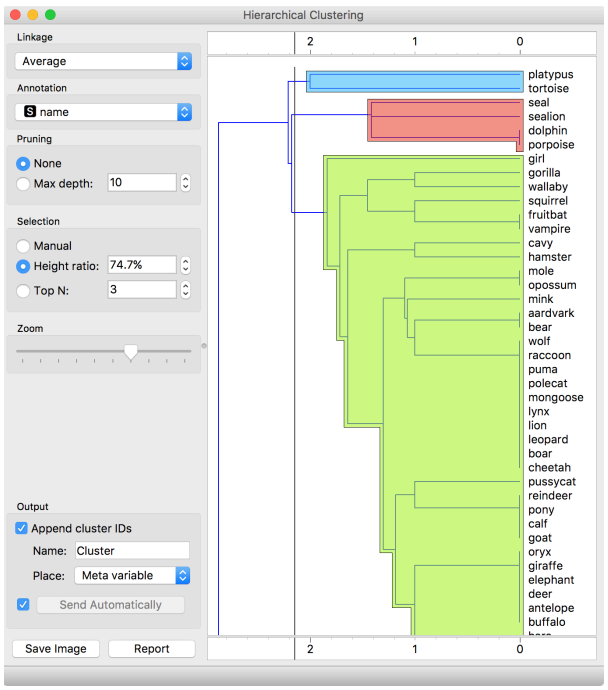
You can also observe the properties of the clusters - that is, the average grades in Algebra and English - in the box plot.

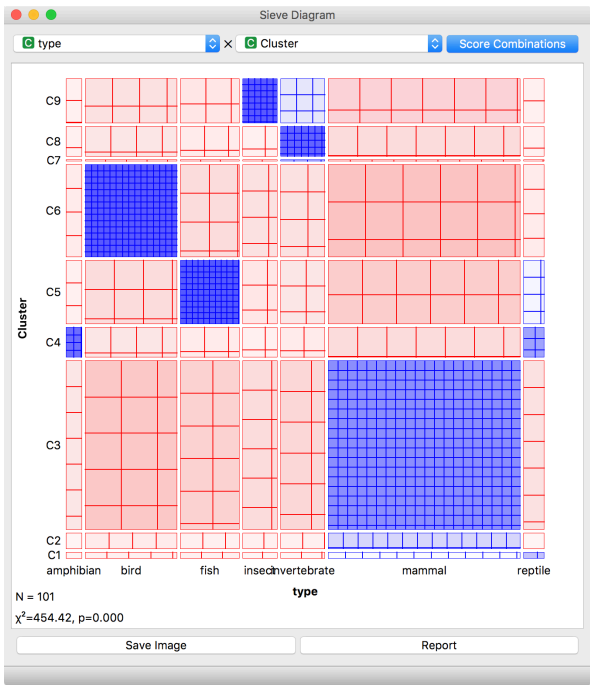
Lesson 27: Animal Kingdom

Your lecturers spent substantial part of their youth admiring a particular Croatian chocolate called Animal Kingdom. Each chocolate bar came with a card — a drawing of some (random) animal, and the associated album made us eat a lot of chocolate. Then our kids came, and the story repeated. Some things stay forever. Funny stuff was we never understood the order in which the cards were laid out in the album. We later learned about taxonomy, but being more inclined to engineering we never mastered learning it in our biology classes. Luckily, there's data mining and the idea that taxonomy simply stems from measuring the distance between species.



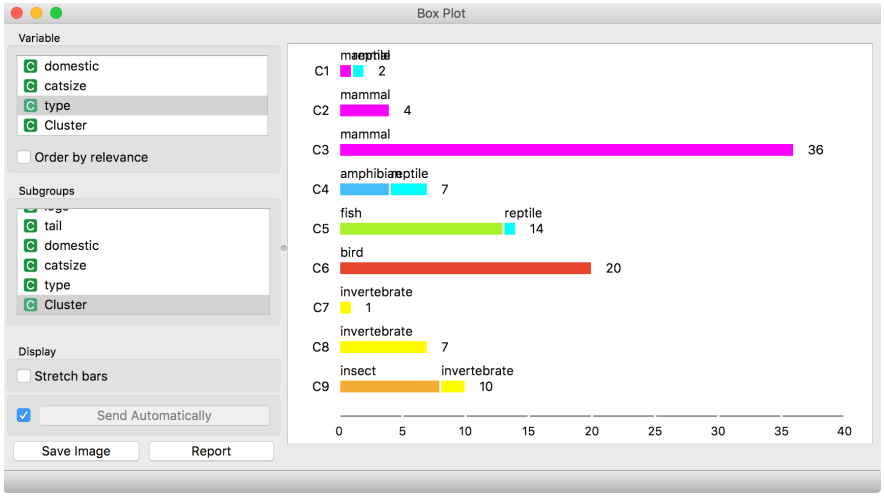
Here we use zoo data (from documentation data sets) with attributes that report on various features of animals (has hair, has feathers, lays eggs). We measure the distance and compute the clustering. Animals in this data set are annotated with type (mammal, insect, bird, and so on). It would be cool to know if the clustering re-discovered these groups of animals. We can do this through marking the clusters in Hierarchical Clustering widget, and then observing the results in the Sieve Diagram.



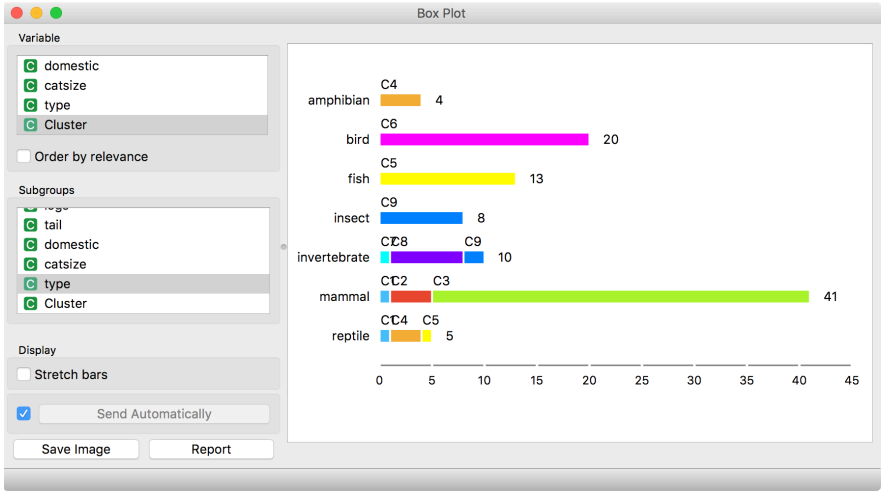


Looks great. Birds, say, are in cluster C6. Cluster C4 consists of amphibians and some reptiles. And so forth.

Checking this in the Box plot is even cooler. We can get a distribution of animal types in each cluster:



Or we can turn it around and see how different types of animals are spread across clusters.



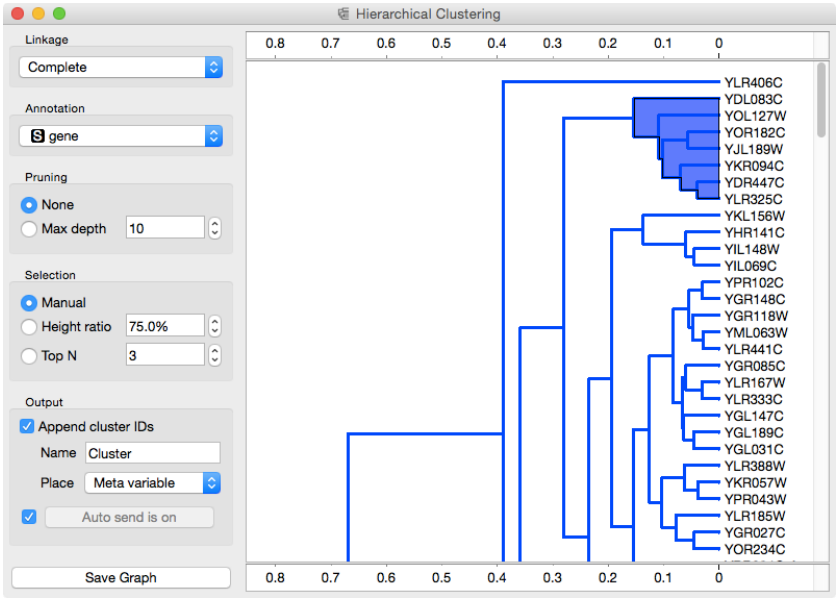
What is wrong with those mammals? Why can't they be in one single cluster? Two reasons. First, they represent 40 % of the data instances. Second, they include some weirdos. Click on the clusters in the box plot and discover who they are.

Lesson 28: Discovering clusters

Can we replicate this on some real data? Can clustering indeed be useful for defining meaningful subgroups?

Take brown-selected (from documentation data sets) connect the hierarchical clustering so the you can see a cluster as a subset in the scatterplot.

So far, we used the dendrogram to set a cut-off point. Now we will click on a branch in a dendrogram to select a subset of the data instances. By combining it with the Scatter Plot widget, we get a great tool for exploring the clusters. Try it with an appropriate pair of features to visualize (use Rank projections).



By using a scatter plot or other widgets, an expert can determine whether the clusters are meaningful.

For this data set, though, we can do something even better. The data already contains some predefined groups. Let us check how

well the clusters match the classes - which we know, but clustering did not.

We will use the dendrogram to set a suitable threshold that splits the data into some three to five clusters. We can plot this data in a new scatter plot; we find a reasonable pair of attributes and then set the color of the points to represent the cluster they belong to. Do the clusters match the actual classes? The result is rather impressive if you keep two things in mind. First, the clustering algorithm did not actually know about the classes, it discovered them by itself. Second, it did not operate on the picture you see in the scatter plot and in which the clusters are quite pronounced, but in a 79-dimensional data space with possibly plenty of redundant features. Yet it identified the three groups of genes almost without mistakes.

This lessons is not a recipe for what you should be doing in practice. If your data already contains groups labels, say gene group annotations, there is no need to discover them (again) by using clustering. In this case you should be interested in predictive models from previous lessons. If you do not have such a grouping but you suspect that the data contains distinct subgroups, run clustering. The sole purpose of this lesson was to demonstrate that clustering can indeed find a meaningful subgroups in the data; we pretend we did not know the groups, use the clustering to discover them, and checked how well the correspond to the actual groups.

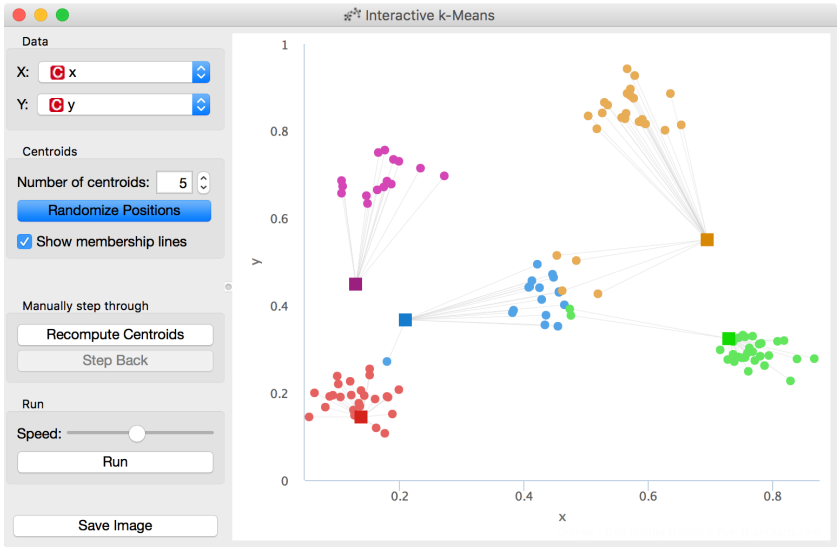
Lesson 29: k-Means Clustering

Hierarchical clustering is not suitable for larger data sets due to the prohibitive size of the distance matrix: with 30 thousand objects, the distance matrix already has almost one billion elements. An alternative approach that avoids using the distance matrix is k-means clustering.

K-means clustering randomly selects k centers (with k specified in advance). Then it alternates between two steps. In one step, it assigns each point to its closest center, thus forming k clusters. In the other, it recomputes the centers of the clusters. Repeating these two steps typically convergences quite fast; even for the big data sets with millions of data points it usually takes just a couple of tens or hundreds iterations.

Orange's add-on Educational provides a widget Interactive k-means, which illustrates the algorithm.

Use the Paint widget to paint some data - maybe five groups of points. Feed it to Interactive k-means and set the number of centroids to 5. You may get something like this.



Try rerunning the clustering from new random positions and observe how the centers conquer the territory. Exciting, isn't it?

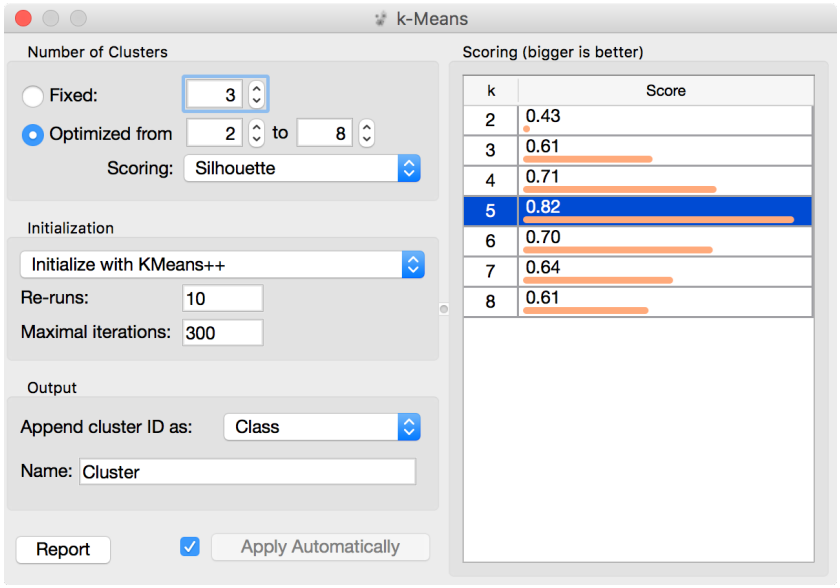
Keep pressing Recompute Centroids and Reassign Membership until it stops changes. With this simple, two-dimensional data it will take just a few iterations; with more points and features, it can take longer, but the principle is the same.

How do we set the initial number of clusters? That's simple: we choose the number that gives the optimal clustering.

Well then, how do we define the optimal clustering? This one is a bit harder. We want small distances between points in the same cluster and large distances between points from different clusters. Pick one point, and let A be its average distance to the data points in the same cluster and let B represent the average distance to the points from the closest other cluster. (The closest cluster? Just compute B for all other clusters and take the lowest value.) The value (B - A) / max(A, B) is called silhouette; the higher the silhouette, the better the point fits into its cluster. The average silhouette across all points is the silhouette of the clustering. The higher the silhouette, the better the clustering.

Now that we can assess the quality of clustering, we can run k-means with different values of parameter k (number of clusters) and select k which gives the largest silhouette.

For this, we abandon our educational toy and connect Paint to the widget k-Means. We tell it to find the optimal number of clusters between 2 and 8, as scored by the Silhouette.



Works like charm.

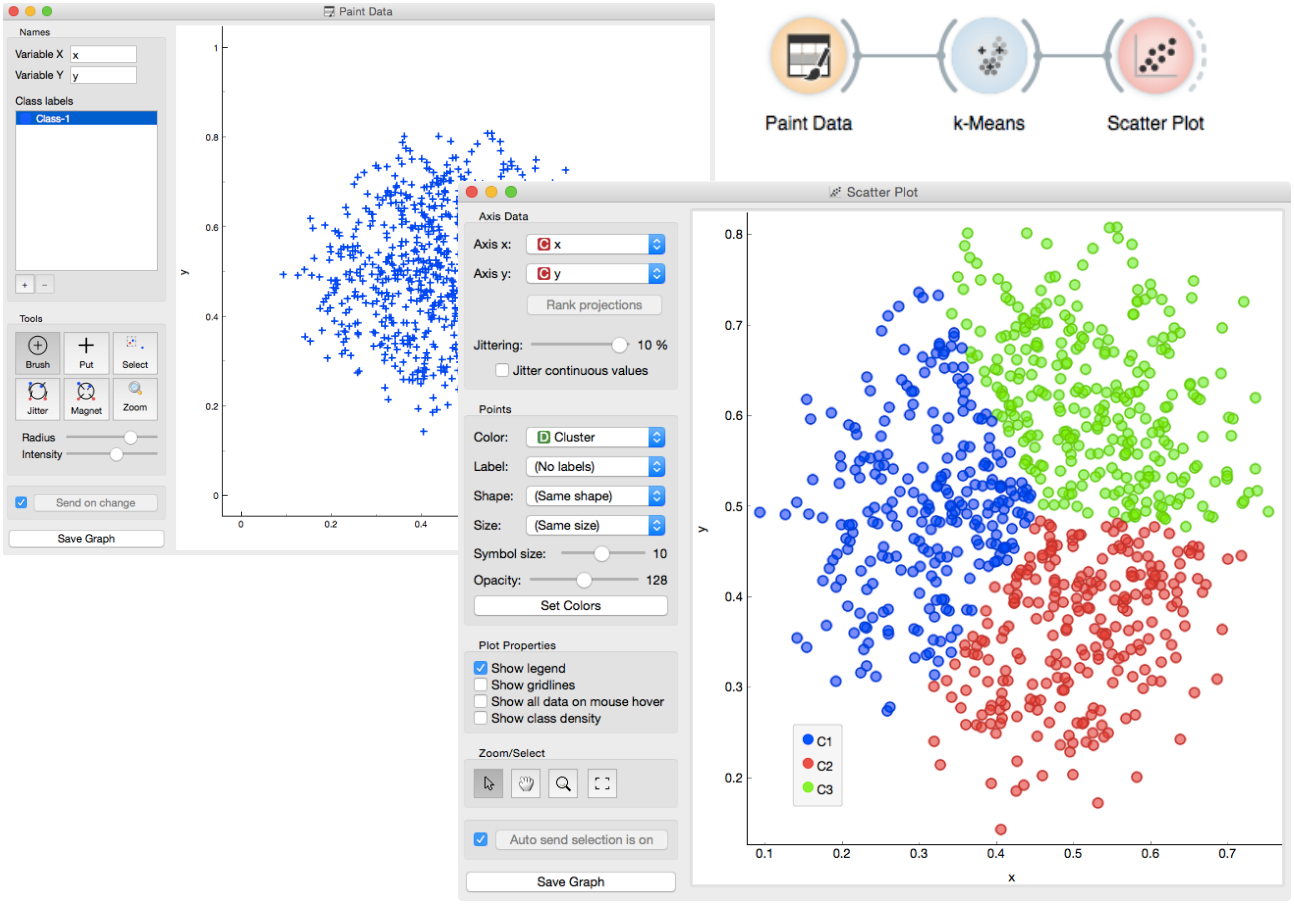
Except that it often doesn't. First, the result of k-means clustering depends on the initial selection of centers. With unfortunate

selection, it may get stuck in a local optimum. We solve this by re-running the clustering multiple times from random positions and using the best result. Second, the silhouette sometimes fails to correctly evaluate the clustering. Nobody's perfect.

Time to experiment. Connect the Scatter Plot to k-Means. Change the number of clusters. See if the clusters make sense. Could you paint the data where k-Means fails? Or where it really works well?

Lesson 30: Finding Clusters When There Are None

We saw how clustering can discover the subgroups in the data. The flip side of this is that algorithms like k-means will always find them even when they do not actually exist.



Playing with Paint Data and k-Means can be quite fun. Try painting the data where there are clusters, but k-means does not find them. Or, actually, finds the wrong ones. What kind of clusters are easy to find for k-means? Are these the kind of clusters we would actually find in real data sets?

It is difficult to verify whether the clusters we found are "real". Data mining methods like clustering can serve only as hints that can help forming new hypotheses, which must make biological sense and be verified on new, independent data. We cannot make conclusions based only on "discovering" clusters.