BIOLAB AND COLLABORATORS

USING ORANGE

BIOLAB

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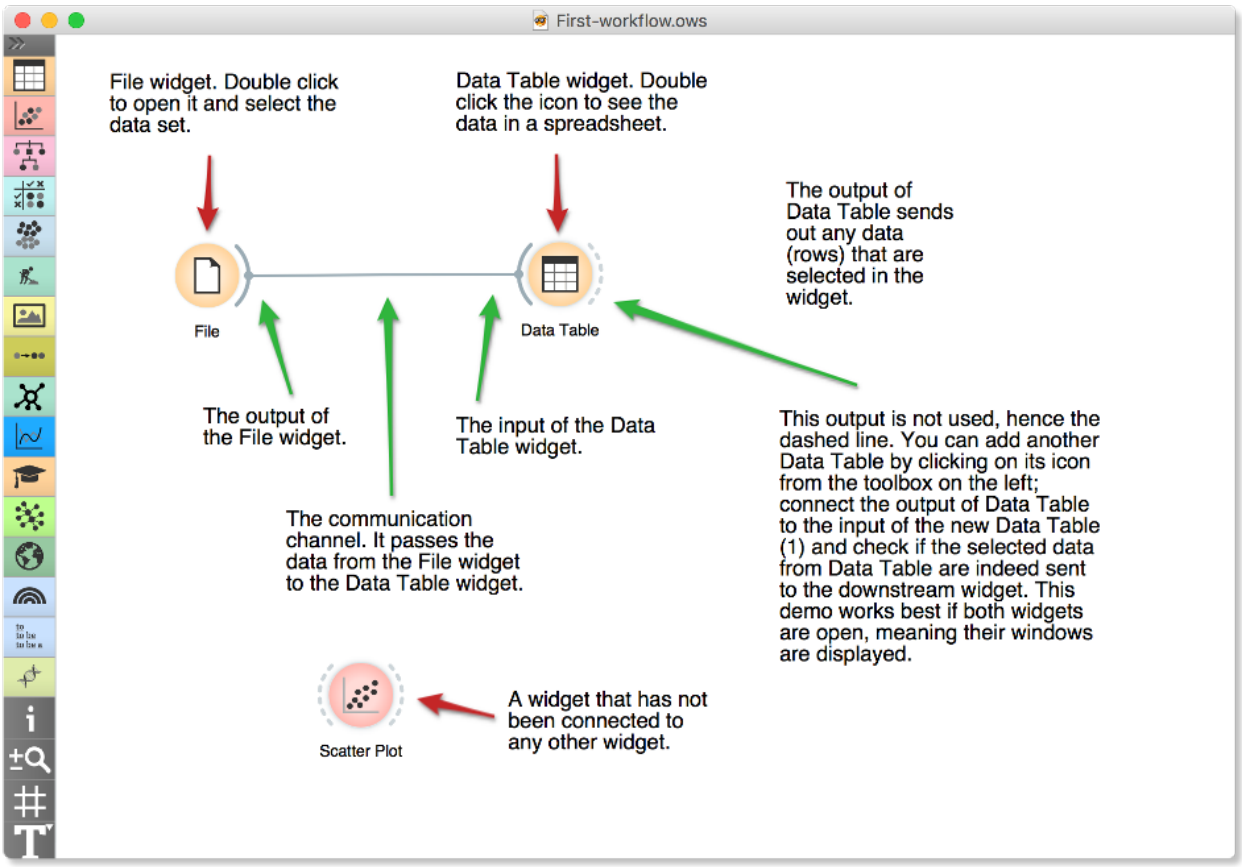
Workflows in Orange

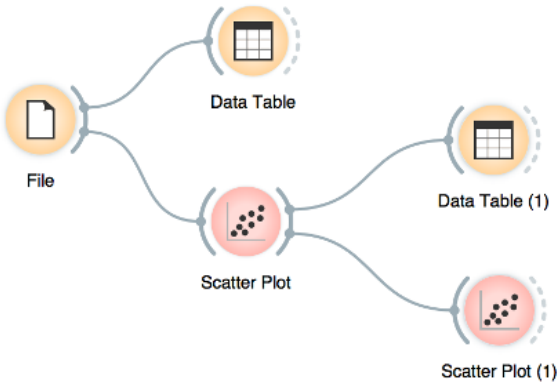
ORANGE WORKFLOWS consist of components that read, process and visualize data. We call them "widgets". Widgets are placed on a drawing board (the "canvas"). Widgets communicate by sending information along a communication channel. Output from one widget is used as input to another.



A simple workflow with two connected widgets and one widget without connections. The outputs of a widget appear on the right, while the inputs appear on the left.

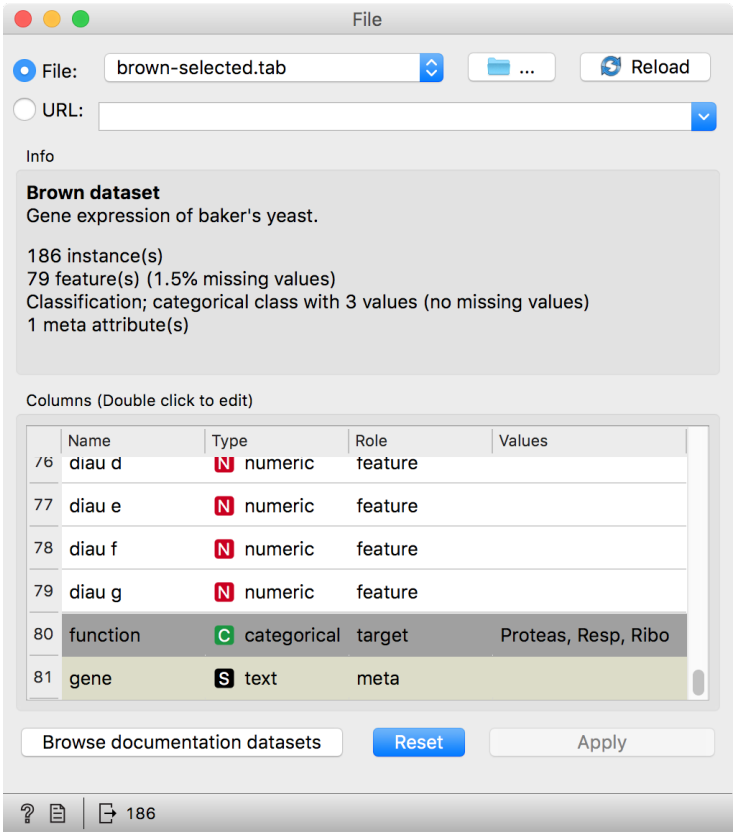
We construct workflows by dragging widgets onto the canvas and connecting them by drawing a line from the transmitting widget to the receiving widget. The widget's outputs are on the right and the inputs on the left. In the workflow above, the *File* widget sends data to the *Data Table* widget.

Start by constructing a workflow that consists of a File widget, two *Scatter Plot* widgets and two Data Table widgets:



Workflow with a File widget that reads the data from a disk and sends it to the Scatter Plot and Data Table widget. The Data Table renders the data in a spreadsheet, while the Scatter Plot visualizes it. Selected data points from the plot are sent to two other widgets: Data Table (1) and Scatter Plot (1).

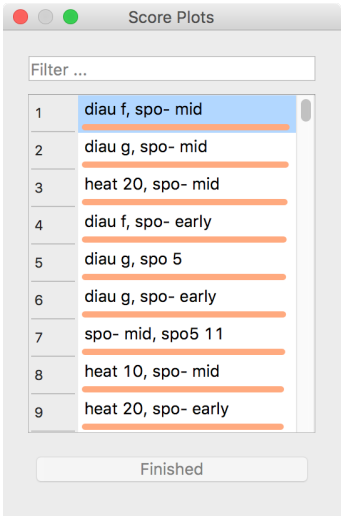
The File widget reads data from your local disk. Open the File widget by double clicking its icon. Orange comes with several preloaded data sets. From these ("Browse documentation data sets. . . "), choose *brown-selected.tab*, a yeast gene expression data set.



Orange workflows often start with a File widget. The brown-selected data set comprises 186 rows (genes) and 81 columns. Out of the 81 columns, 79 contain gene expressions of baker's yeast under various conditions, one column (marked as a "meta attribute") provides gene names, and one column contains the "class" value or gene function.

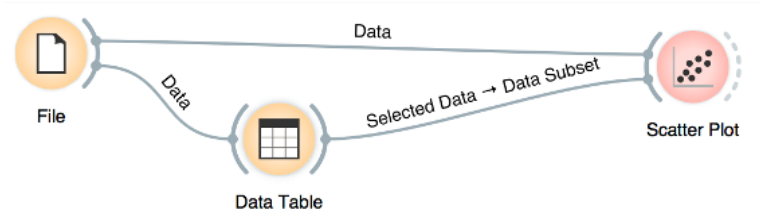
After you load the data, open the other widgets. In the Scatter Plot widget, select a few data points and watch as they appear in the Data Table (1). Use a combination of two Scatter Plot widgets, where the second scatter plot shows a detail from a smaller region selected in the first scatter plot.

The following is more of a side note, but it won't hurt. The scatter plot for a pair of random features does not provide much information on gene function. Does this change with a different choice of feature pairs in the visualization? *Rank projections* (the button on the top left of the Scatter Plot widget) can help you find a good feature pair. How do you think this works? Could the suggested pairs of features be useful to a biologist?



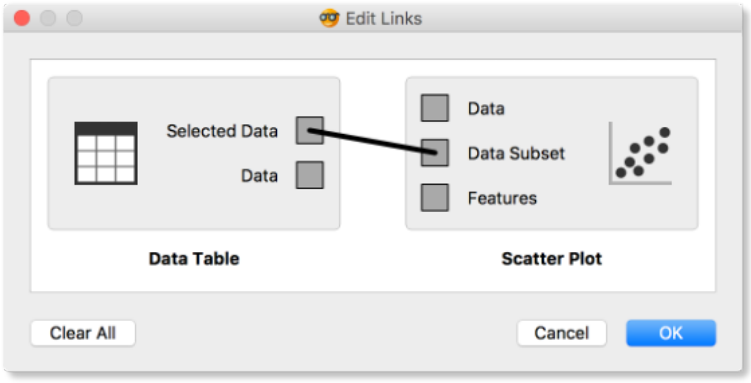
Scatter Plot and Ranking

We can connect the output of the Data Table widget to the Scatter Plot widget to highlight the chosen data instances (rows) in the scatter plot.



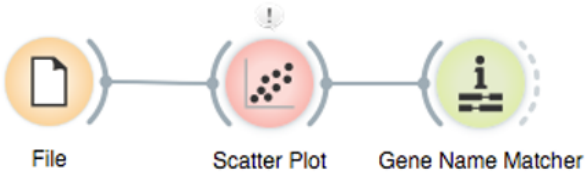
In this workflow, we have switched on the option "Show channel names between widgets" in File/Preferences.

How does Orange distinguish between the primary data source and the data selection? It uses the first connected signal as the entire data set and the second one as its subset. To make changes or to check what is happening under the hood, double click on the line connecting the two widgets.



The rows in the data set we are exploring in this lesson are gene profiles. We could perhaps use widgets from the Bioinformatics add-on to get more information on the genes we selected in any of the Orange widgets.

Orange comes with a basic set of widgets for data input, preprocessing, visualization and modeling. For other tasks, like text mining, network analysis, and bioinformatics, there are add-ons. Check them out by selecting Add-ons... from the Options menu.

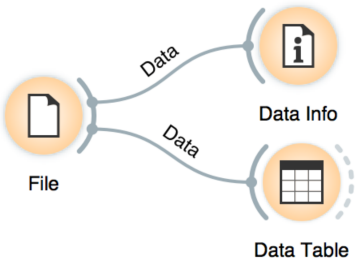


Basic data exploration

Let us consider another problem, this time from clinical medicine. We will dig for something interesting in the data and explore it with visualization widgets. You will get to know Orangebetter, and also learn about several interesting visualizations.

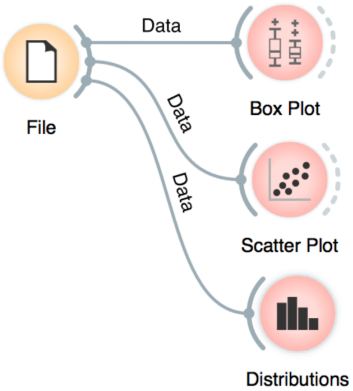
We will start with an empty canvas; to clean it from our previous lesson, use either File/New or select all the widgets and remove them (use the backspace/delete key).

Now again, add the File widget and open another documentation data set: heart_disease. How does the data look like?



A simple workflow to inspect the loaded dataset.

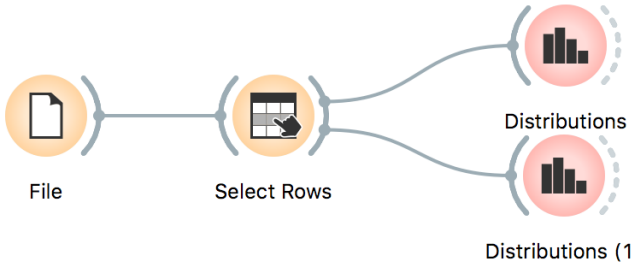
Let us check whether common visualizations tell us anything interesting. (Hint: look for gender differences. These are always interesting and occasionally even real.)



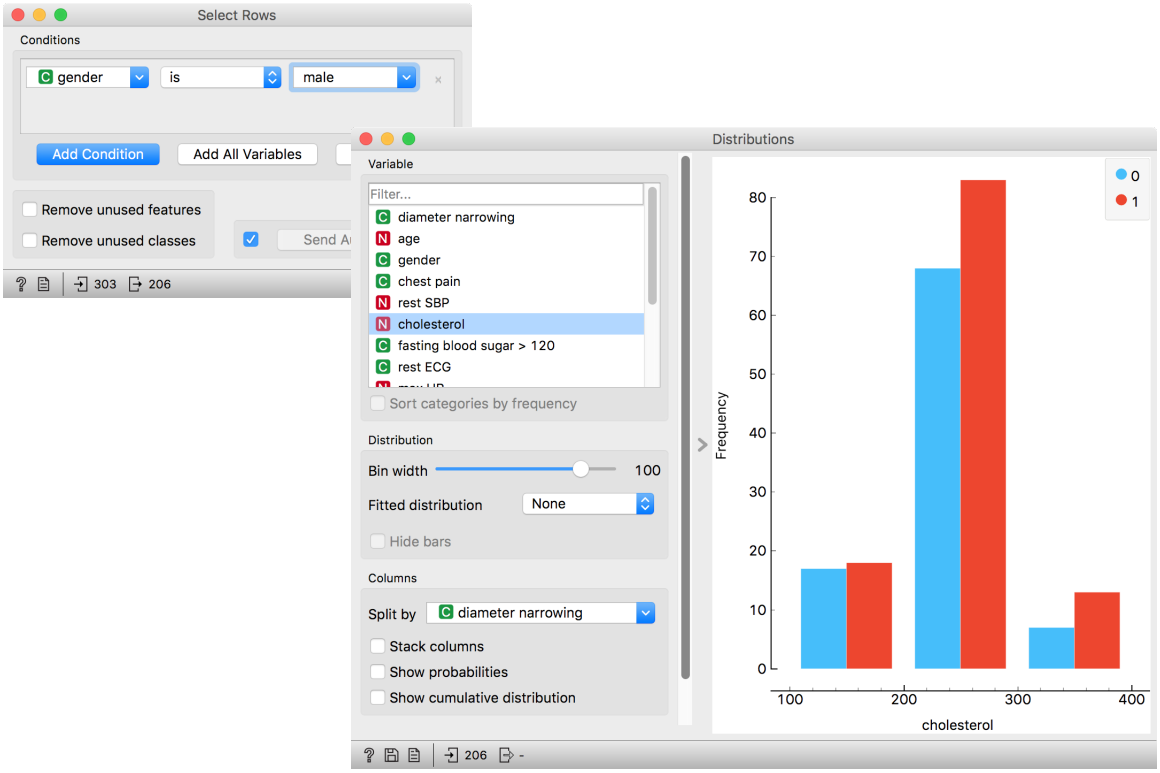
Quick check with common statistics and visualization widgets.

Data can also be split by the value of features, in this case the gender.

The two Distributions widgets get different data: the upper gets the selected rows and the lower gets the rest. Double-click the connection between the widgets to access setup dialog, as you've learned in the previous lesson.



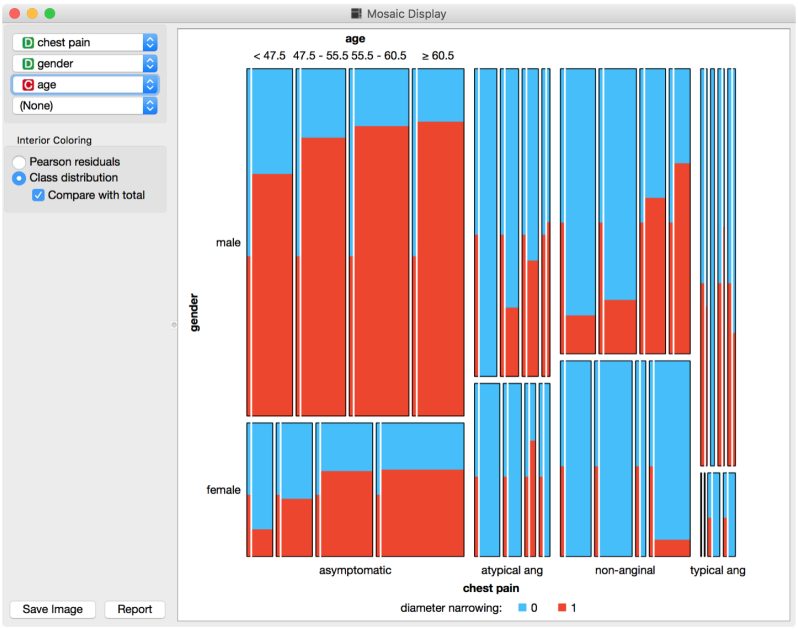
In the Select Rows widget, we select the female patients. You can also add other conditions. Selection of data instances provides a powerful combination with visualization of data distribution. Try having at least two widgets open at the same time and explore the data.



There are two less known — but great — visualizations for observing interactions between features.

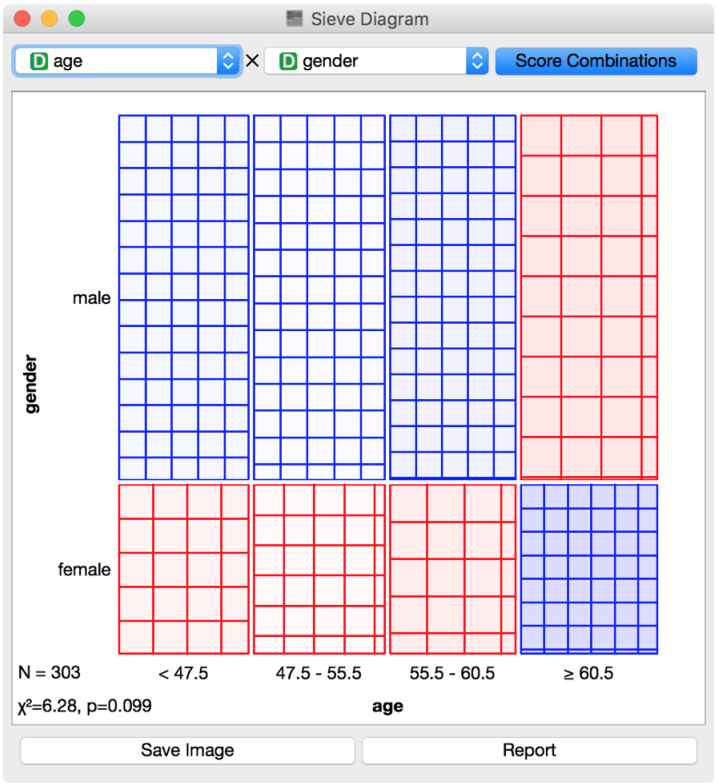
Mosaic display shows a rectangle split into columns with widths reflecting the prevalence of different types of chest pain. Each column is then further split vertically according to gender distributions within the column. The resulting rectangles are split again horizontally according to age group sizes. Within the resulting bars, the red and blue areas represent the outcome distribution for each group and the tiny strip to the left of each shows the overall distribution.

What can you read from this diagram?



You can play with the widget by trying different combinations of 1-4 features.

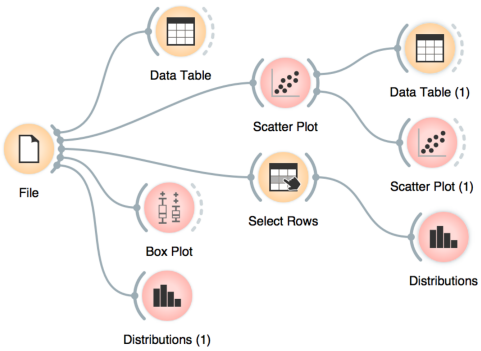
Another visualization, Sieve diagram also splits a rectangle horizontally and vertically, but with independent cuts, so the areas correspond to the expected number of data instances if the observed variables were independent. For instance, 1/4 of patients are older than 60, and 1/3 of patients are female, so the area of the bottom right rectangle is 1/12 of the total area. With roughly 300 patients, we would expect 1/12 × 300 = 25 older women in our data. As a matter of fact, there are 34. Sieve diagram shows the difference between the expected and the observed frequencies by the grid density and the color of the field.



See the Score Combinations button? Guess what it does? And how it scores the combinations? (Hint: there are some Greek letters at the bottom of the widget.)

Saving your work

At the end of a lesson, your workflow may look like this:

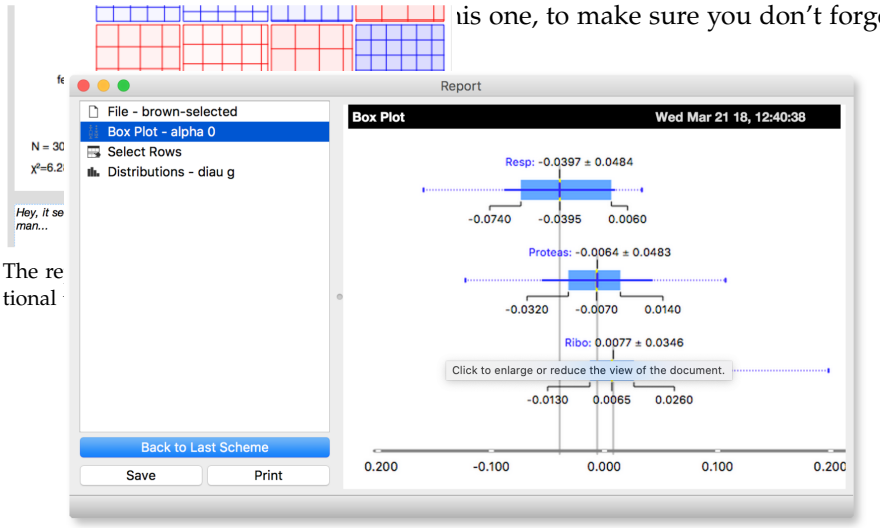


A fairly complex workflow that you would want to share or reuse at a later time.

You can save this workflow, otherwise called a "*Schema*" using the File/Save menu and share it with your colleagues. Just don't forget to put the data files in the same directory as the file with the workflow.

Widgets also have a Report button in their bottom status bar, which you can use to keep a log of your analysis. When you find something interesting, just click it and the graph will be added to your log. You can also add reports from the widgets on the path to this one, to make sure you don't forget anything relevant.

Clicking on a section of the report window allows you to add a comment.

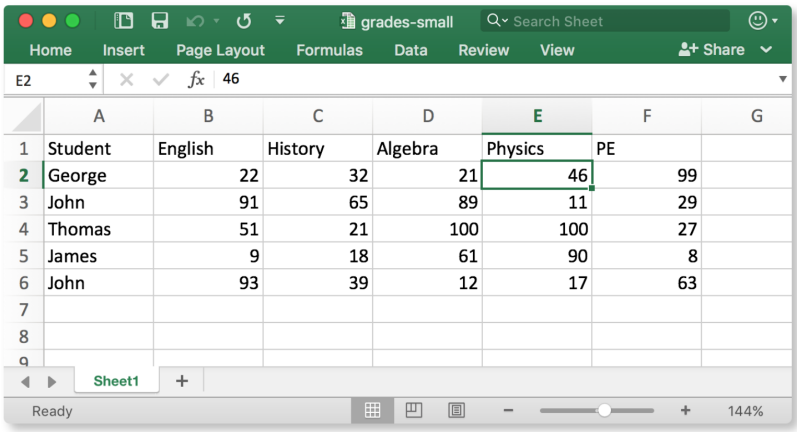


The re
tional

You can save the report as HTML or PDF, or a report file that includes all workflow related report items that you can later open in Orange. In this way, you and your colleagues can reproduce your analysis results.

Loading data sets

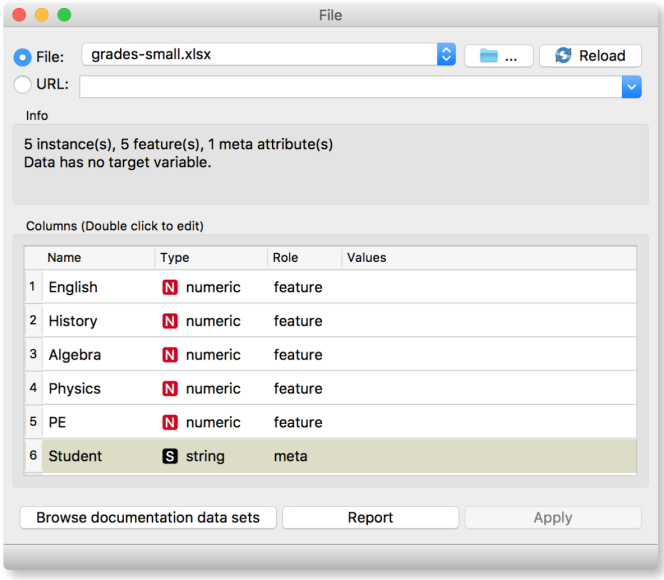
The data sets we have worked with in the previous lesson come with the Orange installation. Orange can read data from many file formats which include tab and comma separated and Excel files. To see how this works, let's prepare a data set (with school subjects and grades) in Excel and save it on a local disk.



	A	B	C	D	E	F	G
1	Student	English	History	Algebra	Physics	PE	
2	George	22	32	21	46	99	
3	John	91	65	89	11	29	
4	Thomas	51	21	100	100	27	
5	James	9	18	61	90	8	
6	John	93	39	12	17	63	
7							
8							

Make a spreadsheet in Excel with the numbers shown on the left. Of course, you can use any other editor, but remember to save your file in the *comma separated values* (*.csv) format.

In Orange, we can use, for example, the File widget to load this data set.



The *File* widget allows you to select a local file or even paste a URL to a Google Spreadsheet. In the Info box, you will see a quick summary about the data you loaded. By double clicking the fields, you can also edit the types of entries and their role, that will be relevant for further processing.

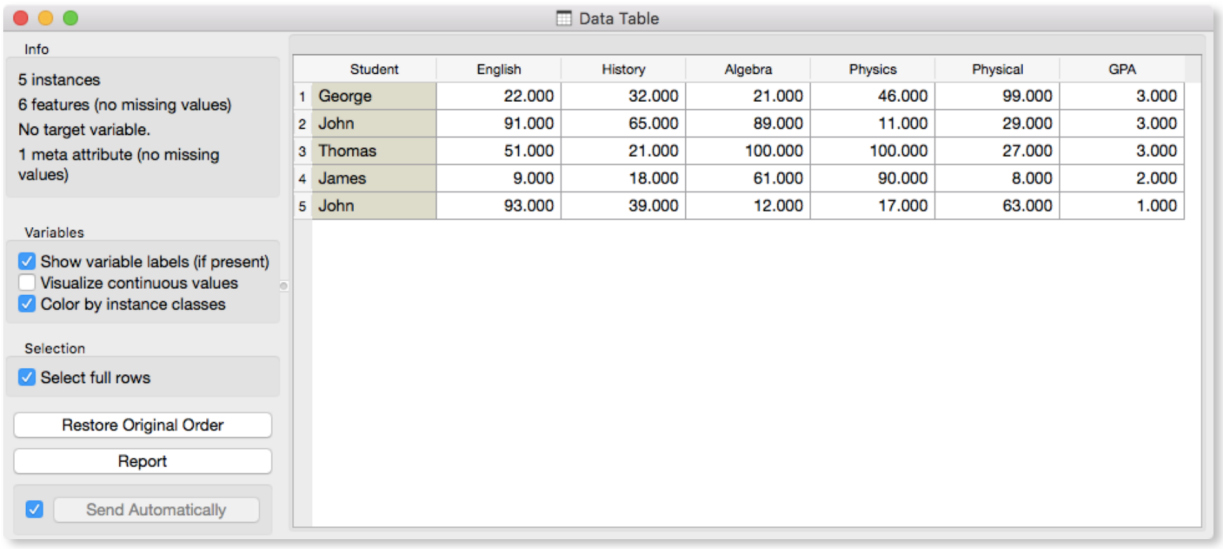
Looks good! Orange has correctly guessed that student names are character strings and that this column in the data set is special,

meant to provide additional information and not to be used for any kind of modeling (more about this in the upcoming lectures). All other columns are numeric features.

It is always good to check if all the data was read correctly. Now, you can connect the *File* widget with the *Data Table* widget,

Make the simple workflow shown on the right.

and double click on the Data Table to see the data in a spreadsheet format. Nice, everything is here.



	Student	English	History	Algebra	Physics	Physical	GPA
1	George	22.000	32.000	21.000	46.000	99.000	3.000
2	John	91.000	65.000	89.000	11.000	29.000	3.000
3	Thomas	51.000	21.000	100.000	100.000	27.000	3.000
4	James	9.000	18.000	61.000	90.000	8.000	2.000
5	John	93.000	39.000	12.000	17.000	63.000	1.000

The *Data Table* widget shows the loaded data set, you can select rows, which will appear on the output of the widget. It is also possible to do simple data visualizations. Explore the functionalities!

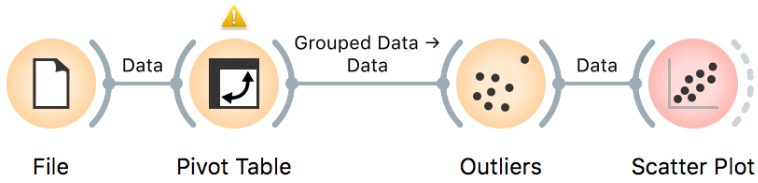
Instead of using Excel, we could also use Google Sheets, a free online spreadsheet alternative. Then, instead of finding the file on the local disk, we would enter its URL address to the File widget URL entry box.

Orange's legacy native data format is a tab-delimited text file with three header rows. The first row lists the attribute names, the second row defines their type (continuous, discrete, time and string, or abbreviated c, d, t, and s), and the third row an optional role (class, meta, weight, or ignore).

There is more to input data formatting and loading. If you would really like to dive in for more, check out the documentation page on Loading your Data, or a video tutorial on this subject.

Assignment: Data Inspection

Understanding the data is crucial for any data science task. And the best way to achieve this is with visualizations. Use FTO3 data from Dr Reddy's and group them by Batch using the Pivot Table widget and its Grouped Data output.



Workflow for the assignment.

1. How are the data distributed? Are there any outlying batches or do they are have a similar range of attributes?
2. Observe the relationship between airflow (airflow. . . actual) and drive speed (drive.speed. . . actual). Is there a categorical variable that nicely splits the data?
3. Try to find an interesting combination of attributes for Sieve Diagram. What does the combination tell you?

Bibliography

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