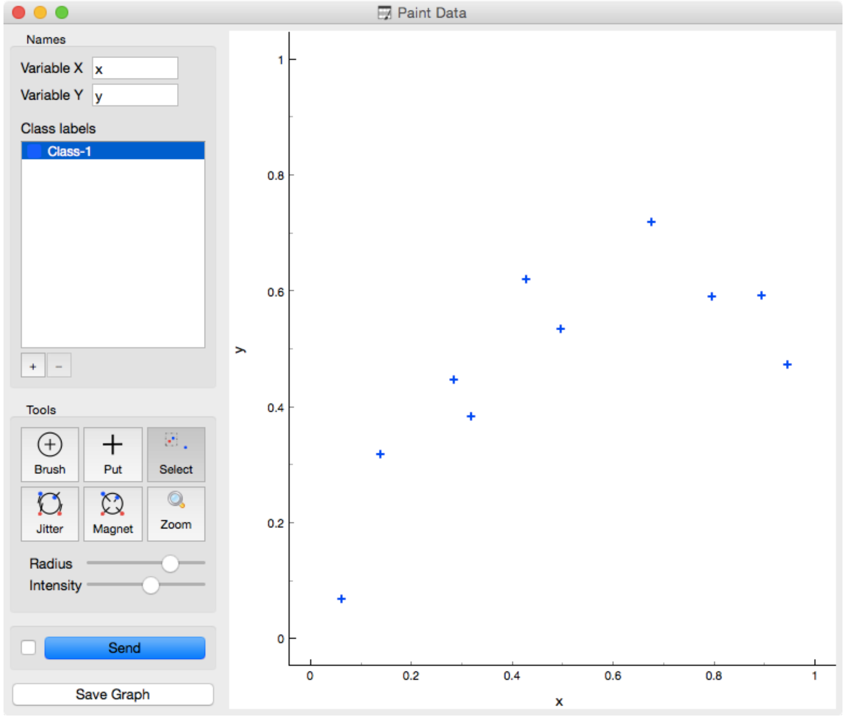
Lesson 9: Linear Regression

For a start, let us construct a very simple data set. It will contain a just one continuous input feature (let's call it *x*) and a continuous class (*y*). We will use Paint Data, and then reassign one of the features to be a class by using Select Column and moving the feature y from the list of "Features" to a field with a target variable. It is always good to check the results, so we are including Data Table and Scatter Plot in the workflow at this stage. We will be modest this time and only paint 10 points and will use Put instead of the Brush tool.

In the Paint Data widget, remove the Class-2 label from the list. If you have accidentally left it while painting, don't despair. The class variable will appear in the Select Columns widget, but you can "remove" it by dragging it into the Available Variables list.



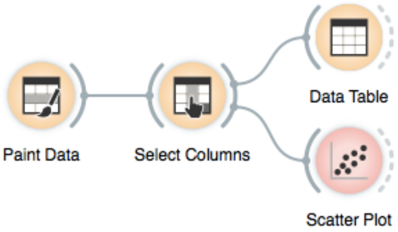
Paint Data

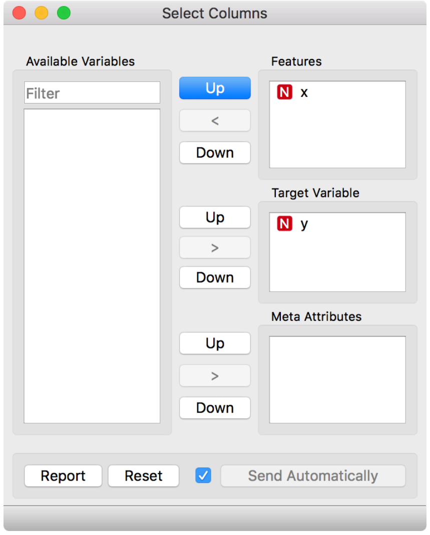
Names

Variable X: x

Variable Y: y

Class labels: Class-1





Select Columns

Available Variables: Filter

Features: N x

Target Variable: N y

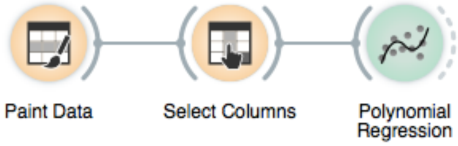
Meta Attributes

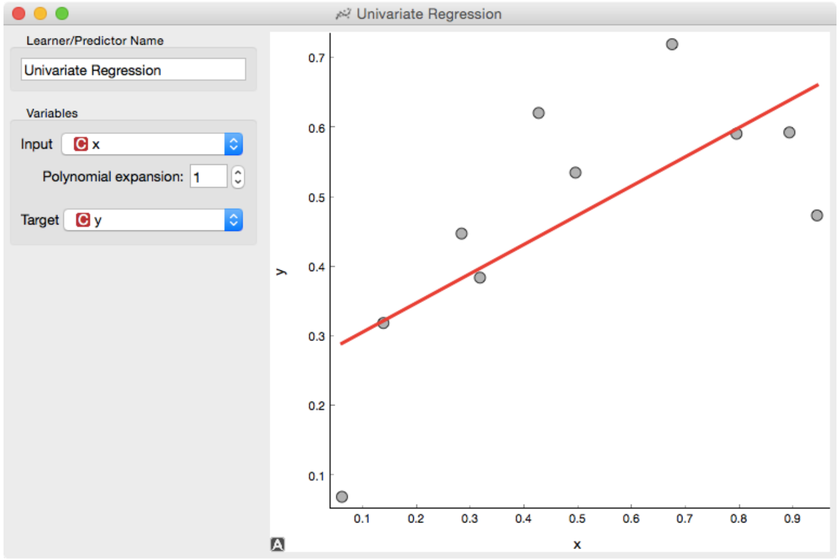
☑ Send Automatically

We would like to build a model that predicts the value of class y from the feature x. Say that we would like our model to be linear, to mathematically express it as $h(x)=\theta_0+\theta_1 x$. Oh, this is the equation of a line. So we would like to draw a line through our data points. The θ_0 is then an intercept, and θ_1 is a slope. But there are many different lines we could draw. Which one is the best one? Which one is the one that is a best fit to our data?

The questions above require us to define what is a good fit. Say, this could be the error the fitted model (the line) makes when it predicts the value of y for a given data point (value of x). The prediction is h(x), so the error is h(x) - y. We should treat the negative and positive errors equally, plus, let us agree, we would prefer punishing larger errors more severely than smaller ones. Therefore, it is perfectly ok if we square the errors for each data point and then sum them up. We got our objective function! Turns out that there is only one line that minimizes this function. The procedure that finds it is called linear regression. For cases where we have only one input feature, Orange has a special widget in the educational add-on called Polynomial Regression.

Do not worry about the strange name of the widget Polynomial Regression, we will get there in a moment.





Learner/Predictor Name

Univariate Regression

Variables

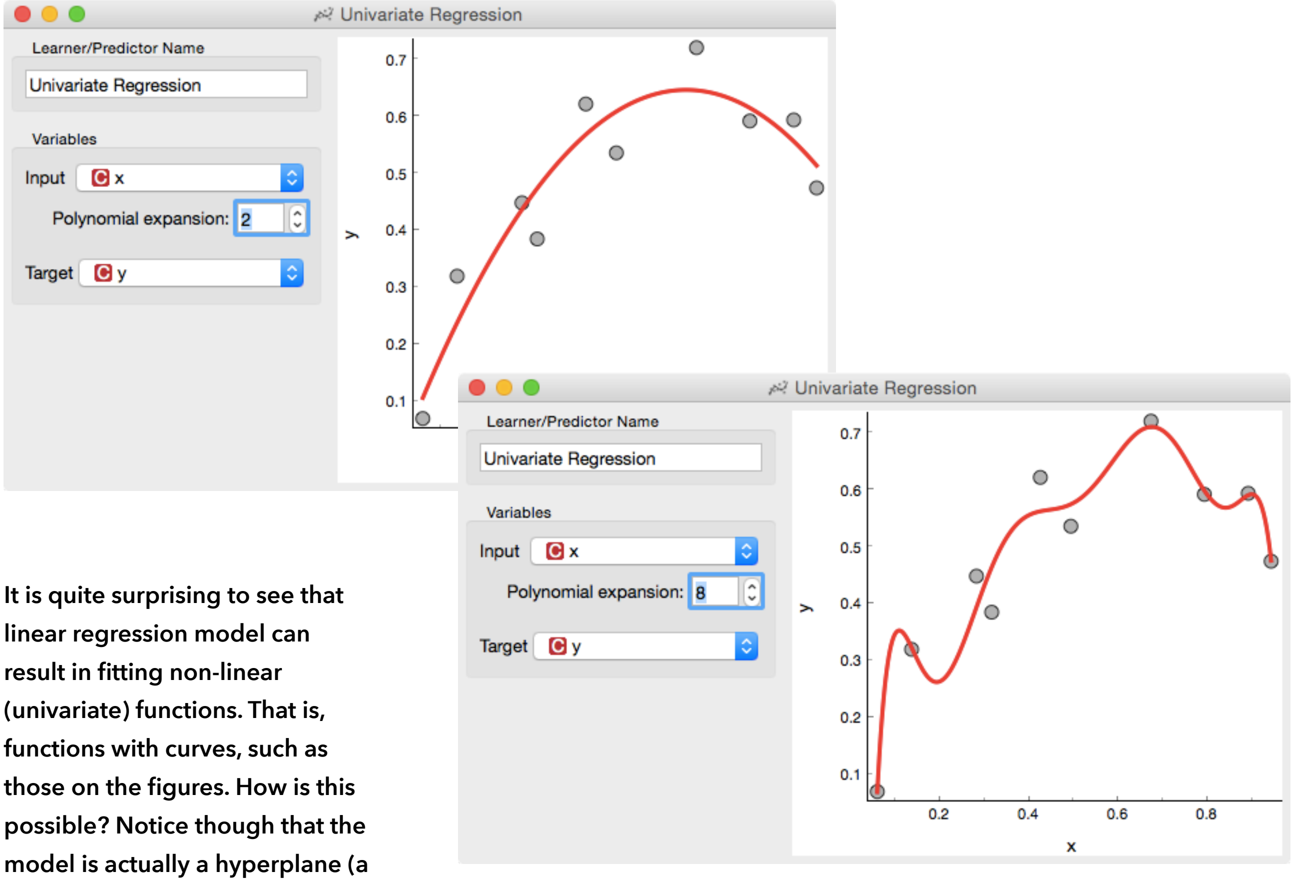
Input: x

Polynomial expansion: 1

Target: y

Looks ok. Except that these data points do not appear exactly on the line. We could say that the linear model is perhaps too simple for our data sets. Here is a trick: besides column x, the widget Univariate Regression can add columns x^2, x^3... x^n to our data set. The number n is a degree of polynomial expansion the widget performs. Try setting this number to higher values, say to two, and then three, and then, say, to nine. With the degree of three, we are then fitting the data to a linear function h(x) = $\theta_0 + \theta_1 x + \theta_1 x^2 + \theta_1 x^3$.

The trick we have just performed (adding the higher order features to the data table and then performing linear regression) is called Polynomial Regression. Hence the name of the widget. We get something reasonable with polynomials of degree two or three, but then the results get really wild. With higher degree polynomials, we totally overfit our data.



Univariate Regression

Learner/Predictor Name: Univariate Regression

Variables

Input: x

Polynomial expansion: 2

Target: y

Univariate Regression

Learner/Predictor Name: Univariate Regression

Variables

Input: x

Polynomial expansion: 8

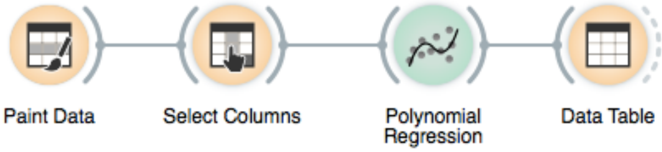
Target: y

It is quite surprising to see that linear regression model can result in fitting non-linear (univariate) functions. That is, functions with curves, such as those on the figures. How is this possible? Notice though that the model is actually a hyperplane (a flat surface) in the space of many features (columns) that are powers of x. So for the degree 2, $\mathrm{h}(x)=\theta_0+\theta_1x+\theta_1x^2$ is a (flat) hyperplane. The visualization gets curvy only once we plot $\mathrm{h}(x)$ as a function of x.

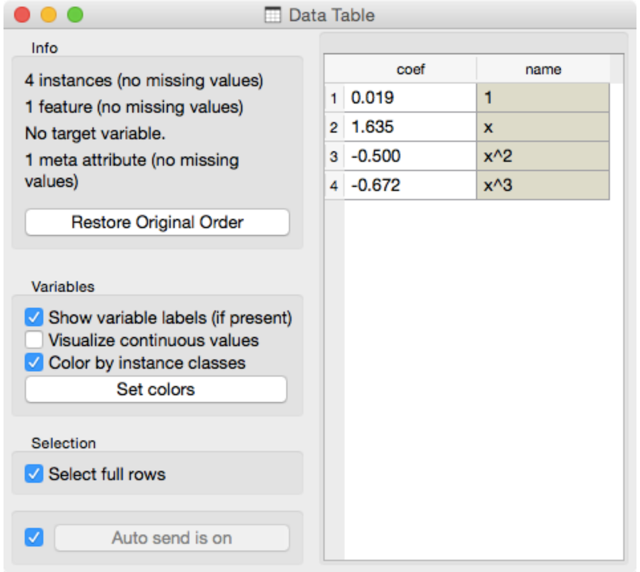
Overfitting is related to the complexity of the model. In polynomial regression, the models are defined through parameters θ. The more parameters, the more complex is the model. Obviously, the simplest model has just one parameter (an intercept), ordinary linear regression has two (an intercept and a slope), and polynomial regression models have as many parameters as is the degree of the polynomial. It is easier to overfit with a more complex model, as this can adjust to the data better. But is the overfitted model really discovering the true data patterns? Which of the two models depicted in the figures above would you trust more?

Lesson 10: Regularization

There has to be some cure for the overfitting. Something that helps us control it. To find it, let's check what the values of the parameters θ under different degrees of polynomials actually are



With smaller degree polynomials values of θ stay small, but then as the degree goes up, the numbers get really large.



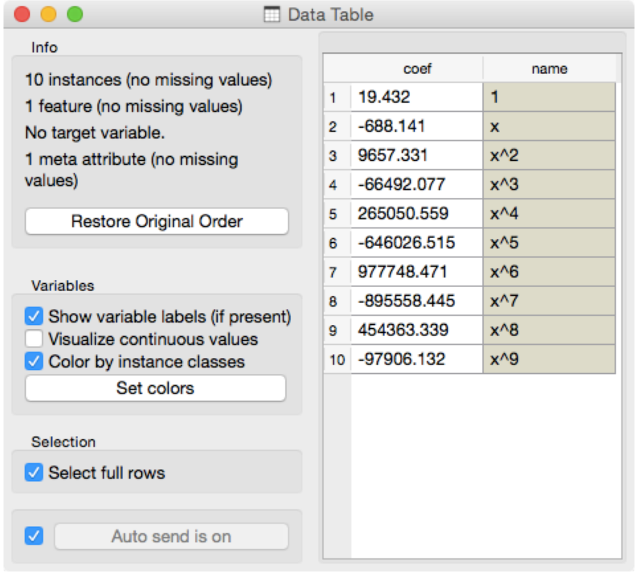
4 instances (no missing values)
1 feature (no missing values)
No target variable.
1 meta attribute (no missing values)

☑ Show variable labels (if present)
□ Visualize continuous values
☑ Color by instance classes

☑ Select full rows

☑ Auto send is on

	coef	name
1	0.019	1
2	1.635	x
3	-0.500	x^2
4	-0.672	x^3



10 instances (no missing values)
1 feature (no missing values)
No target variable.
1 meta attribute (no missing values)

☑ Show variable labels (if present)
□ Visualize continuous values
☑ Color by instance classes

☑ Select full rows

☑ Auto send is on

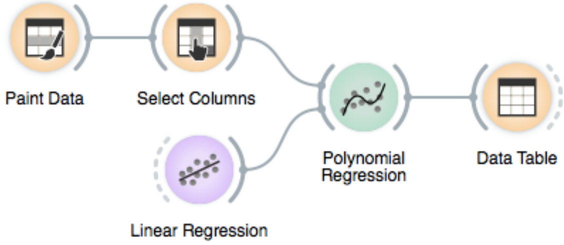
	coef	name
1	19.432	1
2	-688.141	x
3	9657.331	x^2
4	-66492.077	x^3
5	265050.559	x^4
6	-646026.515	x^5
7	977748.471	x^6
8	-895558.445	x^7
9	454363.339	x^8
10	-97906.132	x^9

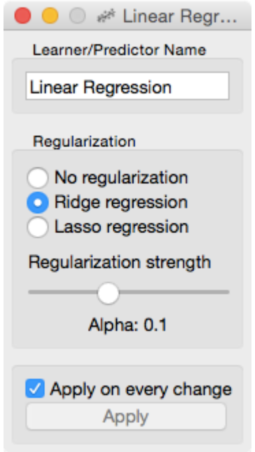
More complex models can fit the training data better. The fitted curve can wiggle sharply. The derivatives of such functions are high, and so need to be the coefficients θ. If only we could force the linear regression to infer models with a small value of coefficients. Oh, but we can. Remember, we have started with the optimization function the linear regression minimizes, the sum of squared errors. We could simply add to this a sum of all θ squared. And ask the linear regression to minimize both terms. Perhaps we should weigh the part with θ squared, say, we some coefficient λ, just to control the level of regularization.

Which inference of linear model would overfit more, the one with high λ or the one with low λ? What should the value of λ be to cancel regularization? What if the value of λ is really high, say 1000?

Internally, if no learner is present on its input, the Polynomial Regression widget would use just its ordinary, non-regularized linear regression.

Here we go: we just reinvented regularization, a procedure that helps machine learning models not to overfit the training data. To observe the effects of the regularization, we can give Polynomial Regression our own learner, which supports these kind of settings.




Linear Regr...

Learner/Predictor Name

Linear Regression

Regularization

○ No regularization
● Ridge regression
○ Lasso regression

Regularization strength

Alpha: 0.1

☑ Apply on every change

Apply

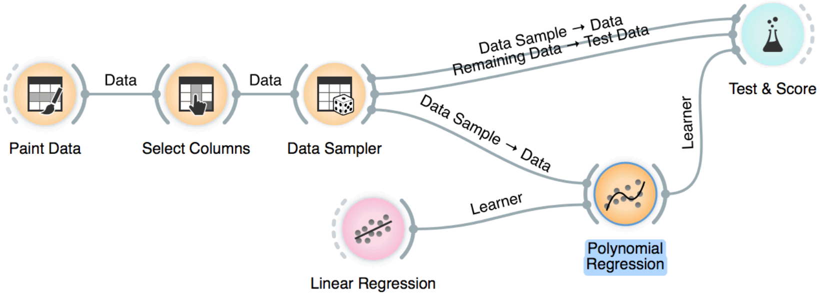
The Linear Regression widget provides two types of regularization. Ridge regression is the one we have talked about and minimizes the sum of squared coefficients θ. Lasso regression minimizes the sum of absolute value of coefficients. Although the difference may seem negligible, the consequences are that lasso regression may result in a large proportion of coefficients θ being zero, in this way performing feature subset selection.

Now for the test. Increase the degree of polynomial to the max. Use Ridge Regression. Does the inferred model overfit the data? How does degree of overfitting depend on regularization strength?

Lesson 11: Regularization and Accuracy on Test Set

Overfitting hurts. Overfit models fit the training data well, but can perform miserably on new data. Let us observe this effect in regression. We will use hand-painted data set, split it into the training (50%) and test (50%) data set, polynomially expand the training data set to enable overfitting, build a model on it, and test the model on both the (seen) training data and the (unseen) held-out data:

Paint about 20 to 30 data instances. Use attribute y as target variable in Select Columns. Split the data 50:50 in Data Sampler. Cycle between test on train or test data in Test & Score. Use ridge regression to build linear regression model.



Now we can vary the regularization strength in Linear Regression and observe the accuracy in Test & Score. For accuracy scoring, we will use RMSE, root mean squared error, which is computed by observing the error for each data point, squaring it, averaging this across all the data instances, and taking a square root. And we will also make use of coefficient of determination, denoted R^2 or r^2, the proportion of the variance in the dependent variable that is predictable from the independent variable(s).

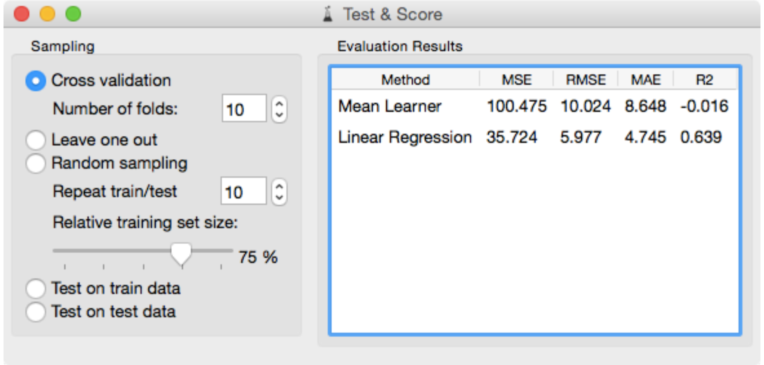
Orange is currently not equipped with parameter fitting and we need to find the optimal level of regularization manually. At this stage, it suffices to say that parameters must be found on the training data set without touching the test data.

The core of this lesson is to compare the error on the training and test set while varying the level of regularization. Remember, regularization controls overfitting - the more we regularize, the less tightly we fit the model to the training data. So for the training set, we expect the error to drop with less regularization and more overfitting, and to increase with more regularization and less fitting. No surprises expected there. But how does this play out on the test set? Which sides minimizes the test-set error? Or is the optimal level of regularization somewhere in between? How do we estimate this level of regularization from the training data alone?

Lesson 12: Prediction of Tissue Age from Level of Methylation

Download the methylation data set from http://file.biolab.si/files/methylation.tab. Predictions of age from methylation profile were investigated by Horvath (2013) Genome Biology 14:R115.

Enough painting. Now for the real data. We will use a data set that includes human tissues from subjects at different age. The tissues were profiled by measurements of DNA methylation, a mechanism for cells to regulate the gene expression. Methylation of DNA is scarce when we are young, and gets more abundant as we age. We have prepared a data set where the degree of methylation was expressed per each gene. Let us test if we can predict the age from the methylation profile - and if we can do this better than by just predicting the average age of subjects in the training set.



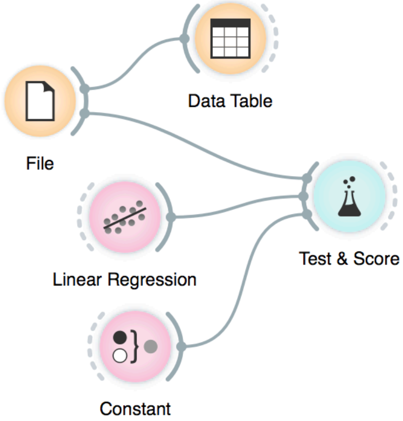
Test & Score

Sampling

- ● Cross validation
  - Number of folds: 10
- ○ Leave one out
- ○ Random sampling
  - Repeat train/test 10
  - Relative training set size: 75 %
- ○ Test on train data
- ○ Test on test data

Evaluation Results

Method	MSE	RMSE	MAE	R2
Mean Learner	100.475	10.024	8.648	-0.016
Linear Regression	35.724	5.977	4.745	0.639



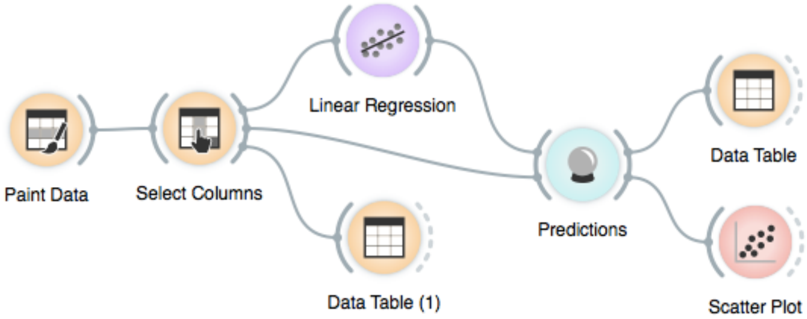
This workflow looks familiar and is similar to those for classification problems. The Test & Score widget reports on statistics we have not seen before. MAE, for one, is the mean average error. Just like for classification, we have used cross-validation, so MAE was computed only on the test data instances and averaged across 10 runs of cross validation. The results indicate that our modeling technique misses the age by about 5 years, which is a much better result than predicting by the mean age in the training set.

Using other learners, like random forests, takes a while on this data set. But you may try to sample the features, obtain a smaller data set, and try various regression learners.

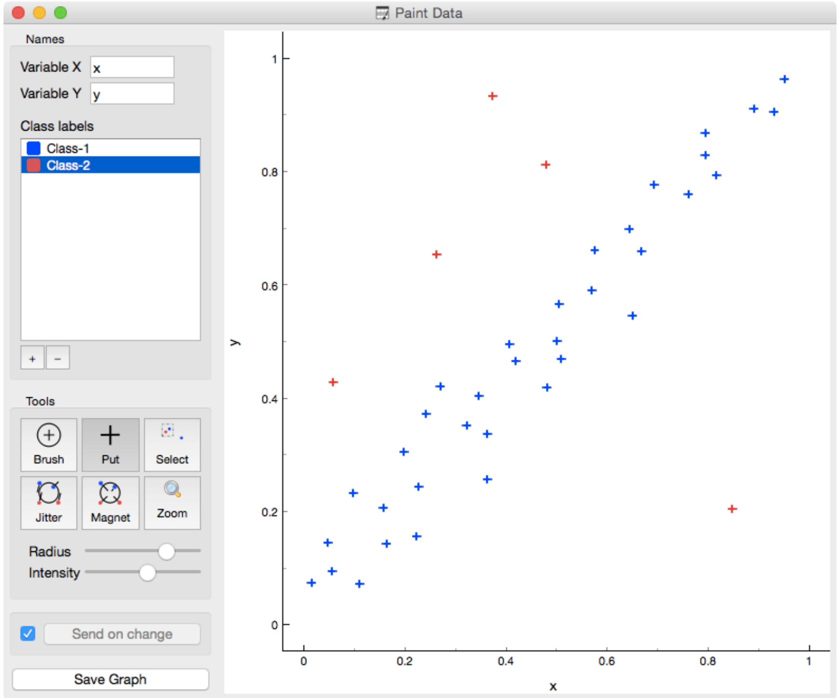
Lesson 13: Evaluating Regression

The last lessons quickly introduced scoring for regression, and important measures such as RMSE and MAE. In classification, a nice addition to find misclassified data instances was the confusion matrix. But the confusion matrix could only be applied to discrete classes. Before Orange gets some similar for regression, one way to find misclassified data instances is through scatter plot!

This workflow visualizes the predictions that were performed on the training data. How would you change the widget to use a separate test set? Hint: The Sample widget can help.



We can play around with this workflow by painting the data such that the regression would perform well on blue data point and fail on the red outliers. In the scatter plot we can check if the difference between the predicted and true class was indeed what we have expected.



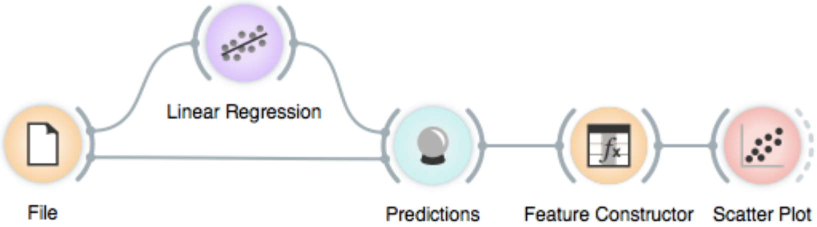
Variable X x

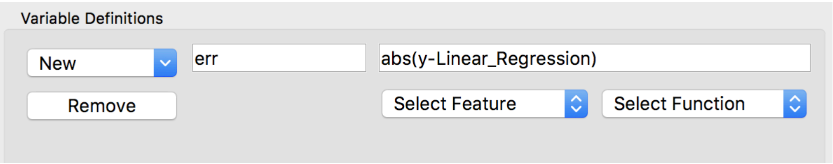
Variable Y y

Class labels: Class-1, Class-2

☑ Send on change

A similar workflow would work for any data set. Take, for instance, the housing data set (from Orange distribution). Say, just like above, we would like to plot the relation between true and predicted continuous class, but would like to add information on the absolute error the predictor makes. Where is the error coming from? We need a new column. The Feature Constructor widget (albeit being a bit geekish) comes to the rescue.





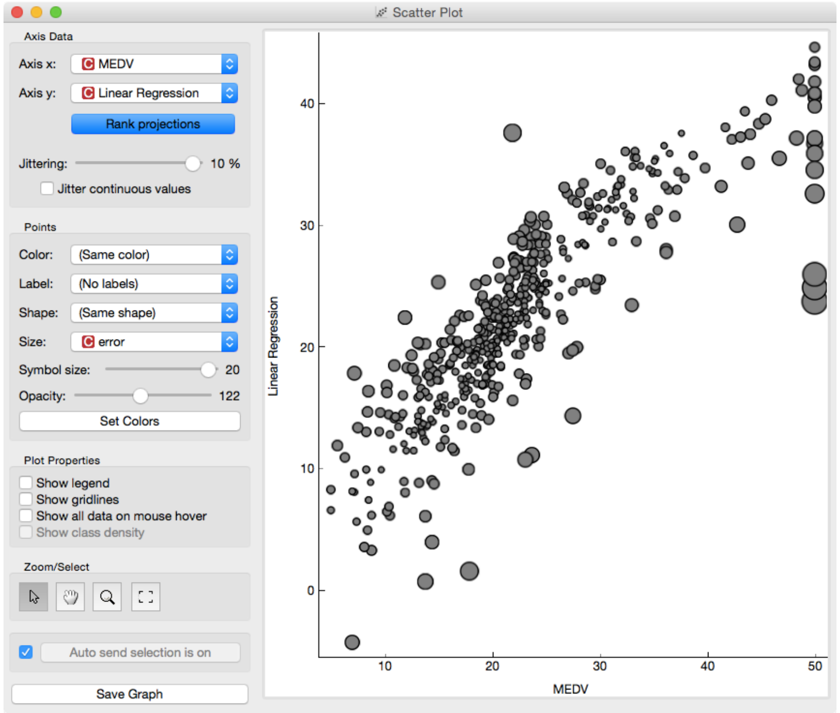
Variable Definitions

New | err | abs(y-Linear_Regression)

Remove | Select Feature | Select Function

In the Scatter Plot widget, we can now select the data where the predictor erred substantially and explore the results further.

We could, in principle, also mine the errors to see if we can identify data instances for which this was high. But then, if this is so, we could have improved predictions at such regions. Like, construct predictors that predict the error. This is weird. Could we then also construct a predictor, that predicts the error of the predictor that predicts the error? Strangely enough, such ideas have recently led to something called Gradient Boosted Trees, which are nowadays among the best regressors (and are coming to Orange soon).



Scatter Plot

Axis Data
Axis x: MEDV
Axis y: Linear Regression
Rank projections
Jittering: 10 %
□ Jitter continuous values

Points
Color: (Same color)
Label: (No labels)
Shape: (Same shape)
Size: error
Symbol size: 20
Opacity: 122
Set Colors

Plot Properties
□ Show legend
□ Show gridlines
□ Show all data on mouse hover
□ Show class density

Zoom/Select

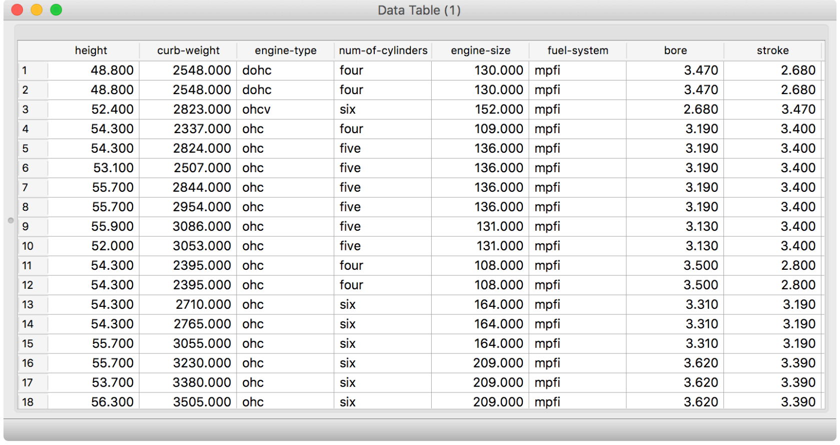
☑ Auto send selection is on

Save Graph

Lesson 14: Feature Scoring and Selection

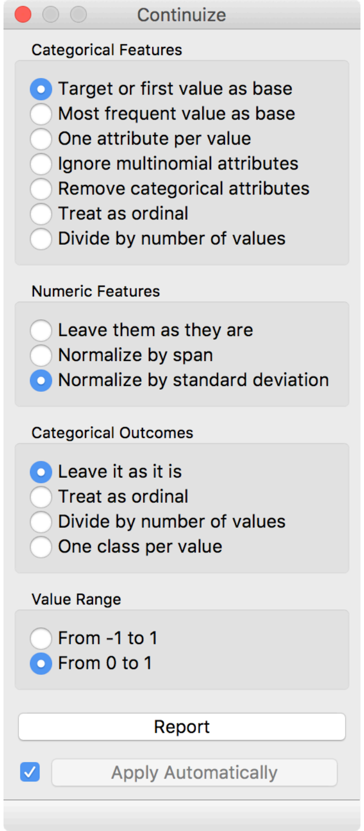
For this lesson, load the data from imports-85.tab using the File widget and Browse documentation data sets.

Linear regression infers a model that estimate the class, a real-valued feature, as a sum of products of input features and their weights. Consider the data on prices of imported cars in 1985. Inspecting this data set in a Data Table, it shows that some features, like fuel-system, engine-type and many others, are discrete. Linear regression only works with numbers. In Orange, linear regression will automatically convert all discrete values to numbers, most often using several features to represent a single discrete features. We also do this conversion manually by using Continuize widget.



Data Table (1)

	height	curb-weight	engine-type	num-of-cylinders	engine-size	fuel-system	bore	stroke
1	48.800	2548.000	dohc	four	130.000	mpfi	3.470	2.680
2	48.800	2548.000	dohc	four	130.000	mpfi	3.470	2.680
3	52.400	2823.000	ohcv	six	152.000	mpfi	2.680	3.470
4	54.300	2337.000	ohc	four	109.000	mpfi	3.190	3.400
5	54.300	2824.000	ohc	five	136.000	mpfi	3.190	3.400
6	53.100	2507.000	ohc	five	136.000	mpfi	3.190	3.400
7	55.700	2844.000	ohc	five	136.000	mpfi	3.190	3.400
8	55.700	2954.000	ohc	five	136.000	mpfi	3.190	3.400
9	55.900	3086.000	ohc	five	131.000	mpfi	3.130	3.400
10	52.000	3053.000	ohc	five	131.000	mpfi	3.130	3.400
11	54.300	2395.000	ohc	four	108.000	mpfi	3.500	2.800
12	54.300	2395.000	ohc	four	108.000	mpfi	3.500	2.800
13	54.300	2710.000	ohc	six	164.000	mpfi	3.310	3.190
14	54.300	2765.000	ohc	six	164.000	mpfi	3.310	3.190
15	55.700	3055.000	ohc	six	164.000	mpfi	3.310	3.190
16	55.700	3230.000	ohc	six	209.000	mpfi	3.620	3.390
17	53.700	3380.000	ohc	six	209.000	mpfi	3.620	3.390
18	56.300	3505.000	ohc	six	209.000	mpfi	3.620	3.390



Continuize

Categorical Features

- ● Target or first value as base
- ○ Most frequent value as base
- ○ One attribute per value
- ○ Ignore multinomial attributes
- ○ Remove categorical attributes
- ○ Treat as ordinal
- ○ Divide by number of values

Numeric Features

- ○ Leave them as they are
- ○ Normalize by span
- ● Normalize by standard deviation

Categorical Outcomes

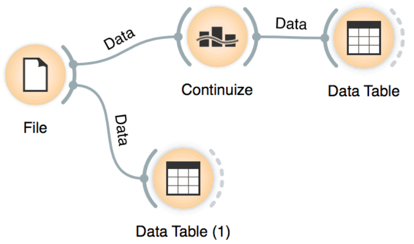
- ● Leave it as it is
- ○ Treat as ordinal
- ○ Divide by number of values
- ○ One class per value

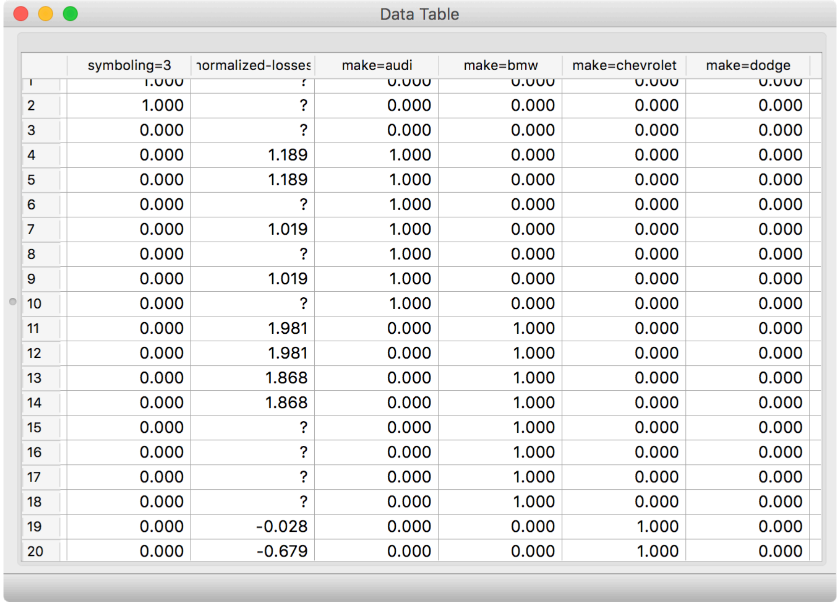
Value Range

- ○ From -1 to 1
- ● From 0 to 1

☑ Apply Automatically

Before we continue, you should check what Continuize actually does and how it converts the nominal features into real-valued features. The table below should provide sufficient illustration.

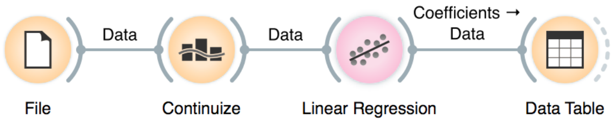


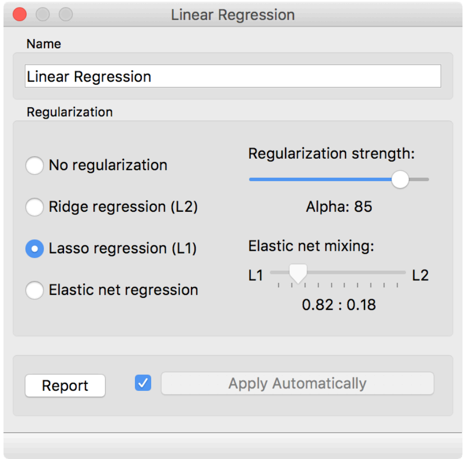


Data Table

	symboling=3	ıormalized-losses	make=audi	make=bmw	make=chevrolet	make=dodge
1	1.000	?	0.000	0.000	0.000	0.000
2	1.000	?	0.000	0.000	0.000	0.000
3	0.000	?	0.000	0.000	0.000	0.000
4	0.000	1.189	1.000	0.000	0.000	0.000
5	0.000	1.189	1.000	0.000	0.000	0.000
6	0.000	?	1.000	0.000	0.000	0.000
7	0.000	1.019	1.000	0.000	0.000	0.000
8	0.000	?	1.000	0.000	0.000	0.000
9	0.000	1.019	1.000	0.000	0.000	0.000
10	0.000	?	1.000	0.000	0.000	0.000
11	0.000	1.981	0.000	1.000	0.000	0.000
12	0.000	1.981	0.000	1.000	0.000	0.000
13	0.000	1.868	0.000	1.000	0.000	0.000
14	0.000	1.868	0.000	1.000	0.000	0.000
15	0.000	?	0.000	1.000	0.000	0.000
16	0.000	?	0.000	1.000	0.000	0.000
17	0.000	?	0.000	1.000	0.000	0.000
18	0.000	?	0.000	1.000	0.000	0.000
19	0.000	-0.028	0.000	0.000	1.000	0.000
20	0.000	-0.679	0.000	0.000	1.000	0.000

Now to the core of this lesson. Our workflow reads the data, coninuizes it such that we also normalize all the features to bring them the to equal scale, then we load the data into Linear Regression widget and check out the feature coefficients in the Data Table.




Linear Regression

Name: Linear Regression

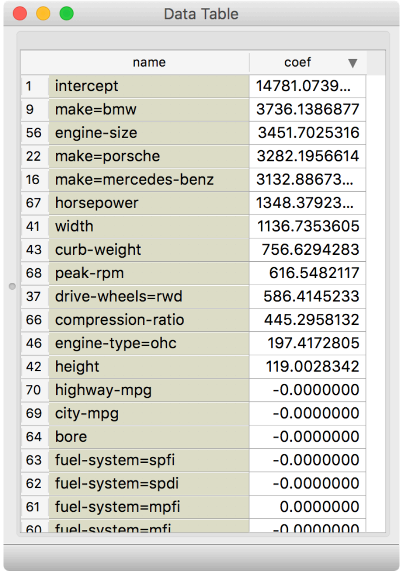
Regularization

○ No regularization
○ Ridge regression (L2)
● Lasso regression (L1)
○ Elastic net regression

Regularization strength: Alpha: 85

Elastic net mixing: L1 0.82 : 0.18 L2

In Linear Regression, we will use L1 regularization. Compared to L2 regularization, which aims to minimize the sum of squared weights, L1 regularization is more rough and minimizes the sum of absolute values of the weights. The result of this "roughness" is that many of the feature will get zero weights. But this may be also exactly what we want. We want to select only the most important features, and want to see how the model that uses only a smaller subset of features actually behaves. Also, this smaller set of features is ranked. Engine size is a huge factor in pricing of our cars, and so is the make, where Porsche, Mercedes and BMW cost more than other cars (ok, no news here).


Data Table

	name	coef
1	intercept	14781.0739...
9	make=bmw	3736.1386877
56	engine-size	3451.7025316
22	make=porsche	3282.1956614
16	make=mercedes-benz	3132.88673...
67	horsepower	1348.37923...
41	width	1136.7353605
43	curb-weight	756.6294283
68	peak-rpm	616.5482117
37	drive-wheels=rwd	586.4145233
66	compression-ratio	445.2958132
46	engine-type=ohc	197.4172805
42	height	119.0028342
70	highway-mpg	-0.0000000
69	city-mpg	-0.0000000
64	bore	-0.0000000
63	fuel-system=spfi	-0.0000000
62	fuel-system=spdi	-0.0000000
61	fuel-system=mpfi	0.0000000
60	fuel-system=mfi	-0.0000000

We should notice that the number of features with non-zero weights varies with regularization strength. Stronger regularization would result in fewer features with non-zero weights.