```
[1]: # Global imports and settings
     from preamble import *
     %matplotlib inline
     plt.rcParams['savefig.dpi'] = 120 # Use 300 for PDF, 100 for slides
     #InteractiveShell.ast_node_interactivity = "all"
     HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-w
```

```
<IPython.core.display.HTML object>
```

Representing Data and Engineering Features

Categorical Variables

In scikit-learn, all input features have to be numeric.

One-Hot-Encoding (Dummy variables) Convert a feature with c categories to c dummy variables:

Load some data with categorical values

```
[2]: import os
     # The file has no headers naming the columns, so we pass header=None
     # and provide the column names explicitly in "names"
     data = pd.read_csv(
         os.path.join(mglearn.datasets.DATA_FOLDER, "adult.data"), header=None,
         names=['age', 'workclass', 'fnlwgt', 'education',  'education-num',
                'marital-status', 'occupation', 'relationship', 'race', 'gender'
                'capital-gain', 'capital-loss', 'hours-per-week', 'native-countr
                'income'])
     # For illustration purposes, we only select some of the columns:
     data = data[['age', 'workclass', 'education', 'gender', 'hours-per-week',
                  'occupation', 'income']]
     # IPython.display allows nice output formatting within the Jupyter notebook
     display(data.head())
```

```
   age          workclass   education   gender  hours-per-week  \
0   39          State-gov   Bachelors     Male              40
1   50   Self-emp-not-inc   Bachelors     Male              13
2   38            Private     HS-grad     Male              40
3   53            Private        11th     Male              40
4   28            Private   Bachelors   Female              40

           occupation  income
0        Adm-clerical   <=50K
1     Exec-managerial   <=50K
2   Handlers-cleaners   <=50K
3   Handlers-cleaners   <=50K
4      Prof-specialty   <=50K
```

Sanity checking string-encoded categorical data It might be that some people specified gender as “male” and some as “man” by mistake

Check the contents of a column by using the value_counts function of a pandas Series:

```
[3]: print(data.gender.value_counts())
```

```
 Male      21790
 Female    10771
Name: gender, dtype: int64
```

Encoding data in pandas (`get_dummies`) Automatically transforms all columns that have object type (like strings) or are categorical.

```
[4]: print("Original features:\n", list(data.columns), "\n")
     data_dummies = pd.get_dummies(data)
     print("Features after get_dummies:\n", list(data_dummies.columns))
```

```
Original features:
 ['age', 'workclass', 'education', 'gender', 'hours-per-week', 'occupation', 'in

Features after get_dummies:
 ['age', 'hours-per-week', 'workclass_ ?', 'workclass_ Federal-gov', 'workclass_
```

```
[5]: display(data_dummies.head(n=2))
```

```
   age  hours-per-week  workclass_ ?  workclass_ Federal-gov     ...       \
0   39              40             0                       0     ...
1   50              13             0                       0     ...

   occupation_ Tech-support  occupation_ Transport-moving  income_ <=50K  \
0                         0                             0              1
1                         0                             0              1

   income_ >50K
0             0
1             0

[2 rows x 46 columns]
```

Next step: Convert the data_dummies DataFrame into a NumPy array, and then train a machine learning model on it.

Be careful to separate the target variable (which is now encoded in two income columns) from the data before training a model.

```
[6]: # Get only the columns containing features
     # that is all columns from 'age' to 'occupation_ Transport-moving'
     # This range contains all the features but not the target

     features = data_dummies.ix[:, 'age':'occupation_ Transport-moving']
     # extract NumPy arrays
     X = features.values
     y = data_dummies['income_ >50K'].values
     print("X.shape: {}  y.shape: {}".format(X.shape, y.shape))
```

```
X.shape: (32561, 44)  y.shape: (32561,)
```

Now the data is represented in a way that scikit-learn can work with, and we can proceed as usual:

```
[7]: from sklearn.linear_model import LogisticRegression
     from sklearn.model_selection import train_test_split
     X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
     logreg = LogisticRegression()
     logreg.fit(X_train, y_train)
     print("Test score: {:.2f}".format(logreg.score(X_test, y_test)))
```

```
Test score: 0.81
```

Integers can encode categories Categorical variables are sometimes pre-encoded as integers (e.g. 0=green, 1=blue. They should not be encoded as a single continuous variable.

To get around this, you need to convert numeric columns in the DataFrame to strings.

```
[8]: # create a dataframe with an integer feature and a categorical string featu
     demo_df = pd.DataFrame({'Integer Feature': [0, 1, 2, 1],
                             'Categorical Feature': ['socks', 'fox', 'socks', 'b
     display(demo_df)
```

```
  Categorical Feature  Integer Feature
0               socks                0
1                 fox                1
2               socks                2
3                 box                1
```

```
[9]: display(pd.get_dummies(demo_df))
```

```
   Integer Feature  Categorical Feature_box  Categorical Feature_fox  \
0                0                        0                        0
1                1                        0                        1
2                2                        0                        0
3                1                        1                        0

   Categorical Feature_socks
0                          1
1                          0
2                          1
3                          0
```

```
[10]: demo_df['Integer Feature'] = demo_df['Integer Feature'].astype(str)
      display(pd.get_dummies(demo_df, columns=['Integer Feature', 'Categorical F
```

```
   Integer Feature_0  Integer Feature_1  Integer Feature_2  \
0                  1                  0                  0
1                  0                  1                  0
```

2	0	0	1
3	0	1	0

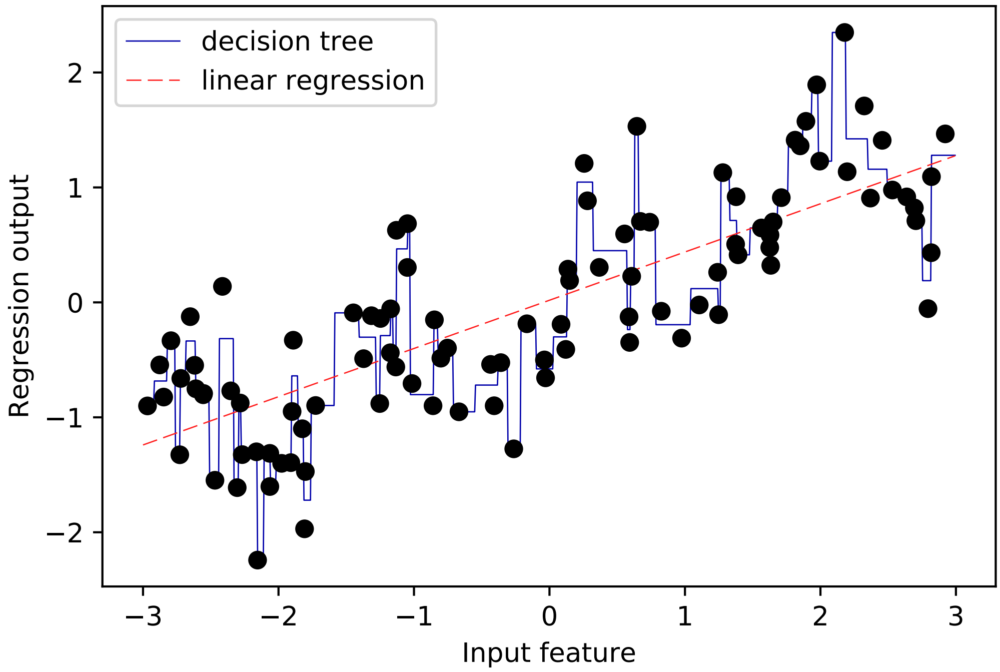
	Categorical Feature_box	Categorical Feature_fox	Categorical Feature_socks
0	0	0	1
1	0	1	0
2	0	0	1
3	1	0	0

Binning (Discretization)

The best way to represent data depends not only on the semantics of the data, but also on the kind of model you are using.
E.g. Linear models can learn better models by using different feature representations.

[11]:
```python
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor

X, y = mglearn.datasets.make_wave(n_samples=100)
line = np.linspace(-3, 3, 1000, endpoint=False).reshape(-1, 1)

reg = DecisionTreeRegressor(min_samples_split=3).fit(X, y)
plt.plot(line, reg.predict(line), label="decision tree")

reg = LinearRegression().fit(X, y)
plt.plot(line, reg.predict(line), label="linear regression")

plt.plot(X[:, 0], y, 'o', c='k')
plt.ylabel("Regression output")
plt.xlabel("Input feature")
plt.legend(loc="best")
```

```
<matplotlib.legend.Legend at 0x1165354e0>
```



Make linear models more powerful by splitting up a feature into multiple artificial features:
- Partition the feature values into a fixed number of bins
- A data point will then be represented by which bin it falls into.

```
[12]: bins = np.linspace(-3, 3, 11)
      print("bins: {}".format(bins))
```

```
bins: [-3.  -2.4 -1.8 -1.2 -0.6  0.   0.6  1.2  1.8  2.4  3. ]
```

Numpy's `digitize` maps each value to its corresponding bin. E.g. the first sample goes to bin nr. 4.

```
[13]: which_bin = np.digitize(X, bins=bins)
      print("\nData points:\n", X[:5])
      print("\nBin membership for data points:\n", which_bin[:5])
```

```
Data points:
 [[-0.753]
 [ 2.704]
 [ 1.392]
 [ 0.592]
 [-2.064]]

Bin membership for data points:
 [[ 4]
 [10]
 [ 8]
 [ 6]
 [ 2]]
```

Encoding data with scikit-learn (`OneHotEncoder`)

- Scikit-learn offers a convenient `OneHotEncoder`
- Call `fit` to compute the internal parameters of the transformation
- Call `transform` to produce the transformed data. You can also run `fit_transform` to do both at once.

!! Test data should *never* be used to compute the preprocessing, because information about the test data will *leak* into the training data, invalidating your model evaluation. Use a nested loop.

```
[14]: from sklearn.preprocessing import OneHotEncoder
      # transform using the OneHotEncoder.
      encoder = OneHotEncoder(sparse=False)
      # encoder.fit finds the unique values that appear in which_bin
      encoder.fit(which_bin)
      # transform creates the one-hot encoding
      X_binned = encoder.transform(which_bin)
      print(X_binned[:5])
```

```
[[0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 [0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]]
```

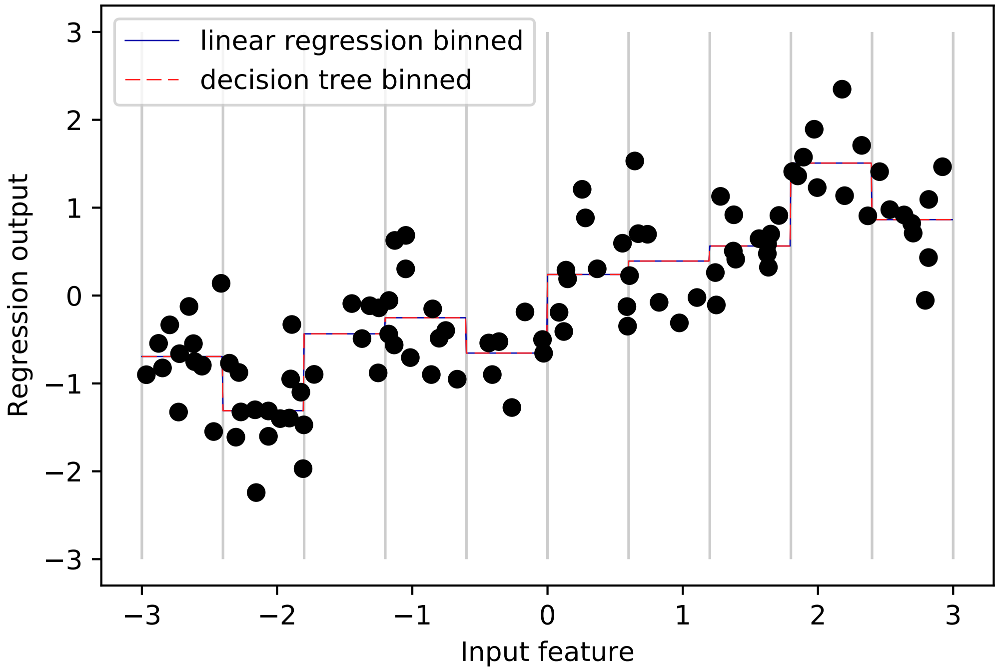
```
[15]: print("X_binned.shape: {}".format(X_binned.shape))
```

```
X_binned.shape: (100, 10)
```

Now we build a new linear regression model and a new decision tree model on the one-hot-encoded data.

```
[16]: line_binned = encoder.transform(np.digitize(line, bins=bins))

      reg = LinearRegression().fit(X_binned, y)
      plt.plot(line, reg.predict(line_binned), label='linear regression binned')

      reg = DecisionTreeRegressor(min_samples_split=3).fit(X_binned, y)
      plt.plot(line, reg.predict(line_binned), label='decision tree binned')
      plt.plot(X[:, 0], y, 'o', c='k')
      plt.vlines(bins, -3, 3, linewidth=1, alpha=.2)
      plt.legend(loc="best")
      plt.ylabel("Regression output")
      plt.xlabel("Input feature")
```

```
<matplotlib.text.Text at 0x1165f8668>
```



Interaction features

Another way to enrich a feature representation, particularly for linear models, is adding interaction features and polynomial features of the original data.

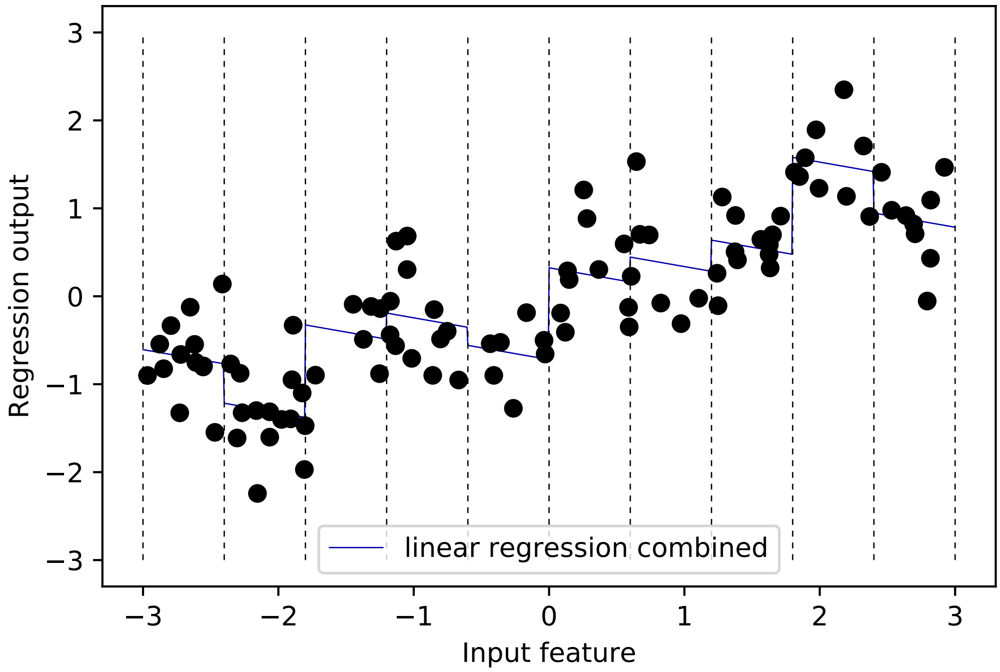
For instance: our linear model learned a constant value for each bin in the wave dataset. If we want a sloped linear model we need to allow interaction with another feature, e.g., the original feature. So let's add the original feature (the x-axis in the plot) back in. This leads to an 11-dimensional dataset:

```
[17]: X_combined = np.hstack([X, X_binned])
      print(X_combined.shape)
```

```
(100, 11)
```

```
[18]: reg = LinearRegression().fit(X_combined, y)

      line_combined = np.hstack([line, line_binned])
      plt.plot(line, reg.predict(line_combined), label='linear regression combin

      for bin in bins:
          plt.plot([bin, bin], [-3, 3], ':', c='k')
      plt.legend(loc="best")
      plt.ylabel("Regression output")
      plt.xlabel("Input feature")
      plt.plot(X[:, 0], y, 'o', c='k')
```

```
[<matplotlib.lines.Line2D at 0x116367d68>]
```



Product features

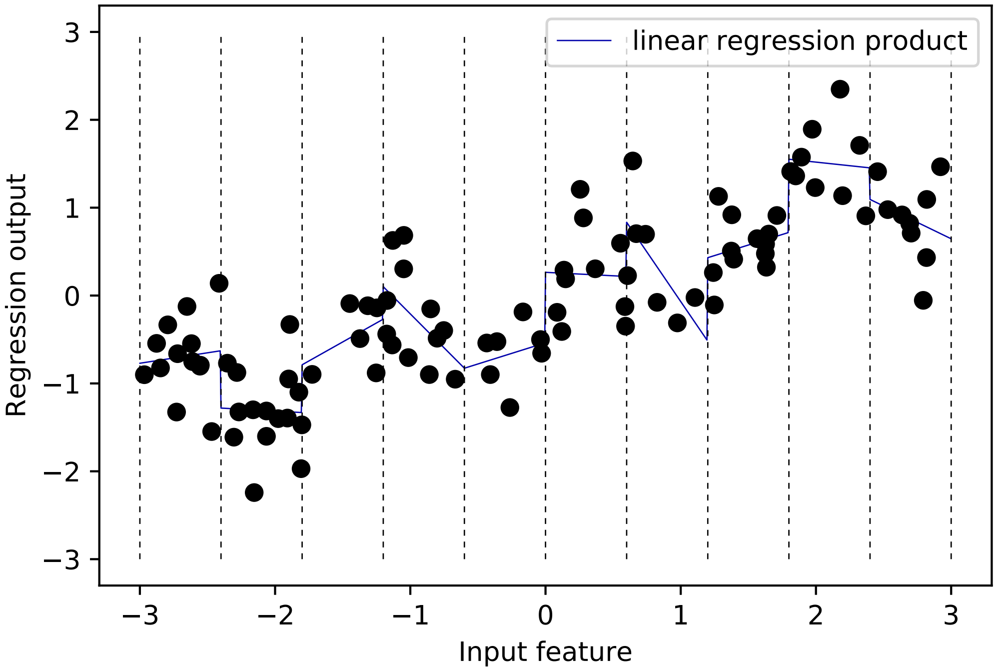
If we want a different slope per bin, we need a new *interaction feature* (or *product feature*) that indicates in which bin a data point is in **and** where it lies on the x-axis.

```
[19]: X_product = np.hstack([X_binned, X * X_binned])
      print(X_product.shape)
```

```
(100, 20)
```

```
[20]: reg = LinearRegression().fit(X_product, y)

      line_product = np.hstack([line_binned, line * line_binned])
      plt.plot(line, reg.predict(line_product), label='linear regression product

      for bin in bins:
          plt.plot([bin, bin], [-3, 3], ':', c='k')

      plt.plot(X[:, 0], y, 'o', c='k')
      plt.ylabel("Regression output")
      plt.xlabel("Input feature")
      plt.legend(loc="best")
```

```
<matplotlib.legend.Legend at 0x11a8cde48>
```



Polynomials

We can also make linear models behave more flexibly by adding polynomials of the original continuous features.

For a given feature x, we might want to consider x^2, x^3, x^4, and so on. In scikit-learn, this is implemented in `PolynomialFeatures` in the preprocessing module

```
[21]: from sklearn.preprocessing import PolynomialFeatures

      # include polynomials up to x ** 10:
      # the default "include_bias=True" adds a features that's constantly 1
      poly = PolynomialFeatures(degree=10, include_bias=False)
      poly.fit(X)
      X_poly = poly.transform(X)
```

Using a degree of 10 yields 10 features, with the original value raised to the n-th power.

```
[22]: print("X_poly.shape: {}".format(X_poly.shape))
```

```
X_poly.shape: (100, 10)
```

```
[23]: print("Entries of X:\n{}".format(X[:5]))
      print("Entries of X_poly:\n{}".format(X_poly[:5]))
```

```
Entries of X:
[[-0.753]
 [ 2.704]
 [ 1.392]
```

```
 [ 0.592]
 [-2.064]]
Entries of X_poly:
[[    -0.753      0.567     -0.427      0.321     -0.242      0.182     -0.137
       0.103     -0.078      0.058]
 [     2.704      7.313     19.777     53.482    144.632    391.125   1057.714
    2860.36    7735.232  20918.278]
 [     1.392      1.938      2.697      3.754      5.226      7.274     10.125
      14.094     19.618     27.307]
 [     0.592      0.35       0.207      0.123      0.073      0.043      0.025
       0.015      0.009      0.005]
 [    -2.064      4.26      -8.791     18.144    -37.448     77.289   -159.516
     329.222   -679.478   1402.367]]
```

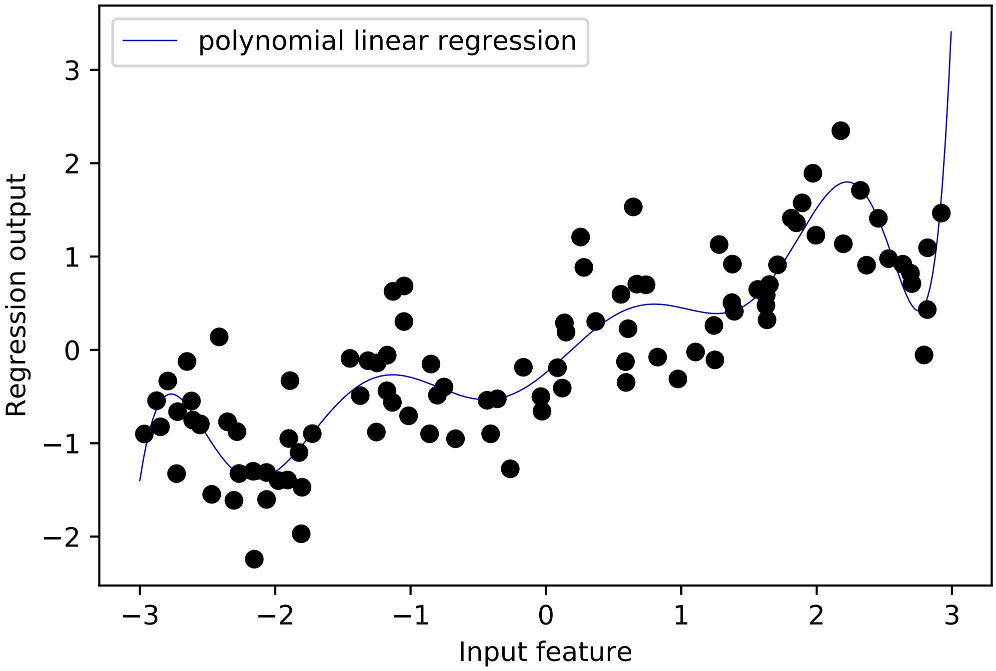
```
[24]: print("Polynomial feature names:\n{}".format(poly.get_feature_names()))
```

```
Polynomial feature names:
['x0', 'x0^2', 'x0^3', 'x0^4', 'x0^5', 'x0^6', 'x0^7', 'x0^8', 'x0^9', 'x0^10']
```

Using polynomial features together with a linear regression model yields *polynomial regression*.

```
[25]: reg = LinearRegression().fit(X_poly, y)

      line_poly = poly.transform(line)
      plt.plot(line, reg.predict(line_poly), label='polynomial linear regression
      plt.plot(X[:, 0], y, 'o', c='k')
      plt.ylabel("Regression output")
      plt.xlabel("Input feature")
      plt.legend(loc="best")
```

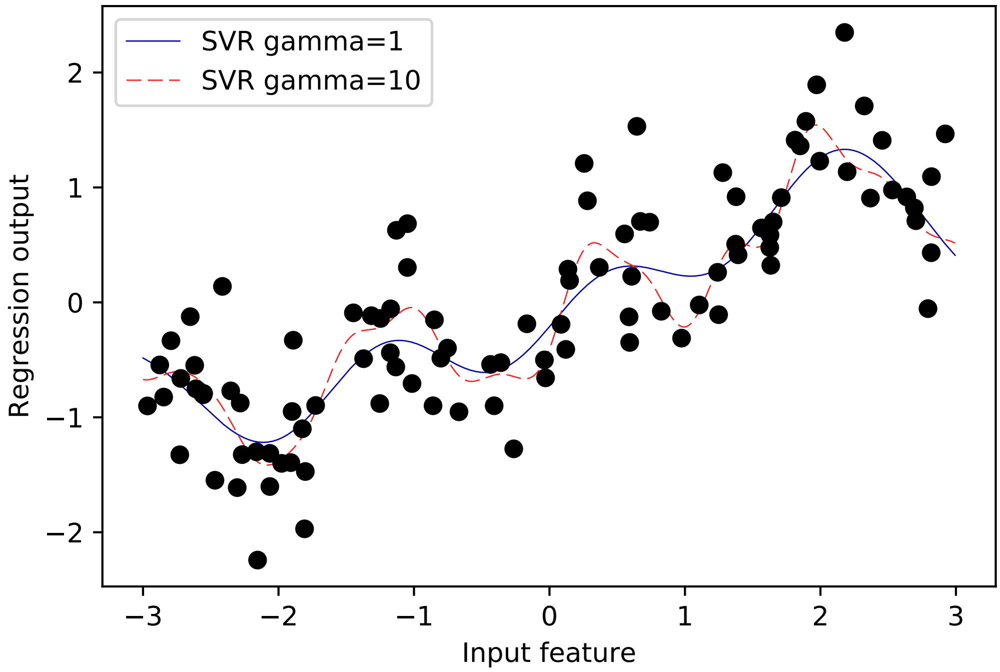
```
<matplotlib.legend.Legend at 0x1163f8ef0>
```



As a comparison, here is a kernel SVM model learned on the original data, without any transformation

```
[26]: from sklearn.svm import SVR

      for gamma in [1, 10]:
          svr = SVR(gamma=gamma).fit(X, y)
          plt.plot(line, svr.predict(line), label='SVR gamma={}'.format(gamma))

      plt.plot(X[:, 0], y, 'o', c='k')
      plt.ylabel("Regression output")
      plt.xlabel("Input feature")
      plt.legend(loc="best")
```

```
<matplotlib.legend.Legend at 0x116418160>
```



Non-linear transformations

There are other transformations that often prove useful for transforming certain features.

For instance, `log` or `exp` are very useful to better scale your data. This is useful for models that are sensitive to feature scales, such as linear models, SVMs and neural networks.

The functions log and exp can help by adjusting the relative scales, tranforming them to more Gaussian-like value distributions.

Here we generate some data that has a very non-normal (Poisson) distribution:

```
[27]: rnd = np.random.RandomState(0)
      X_org = rnd.normal(size=(1000, 3))
      w = rnd.normal(size=3)

      X = rnd.poisson(10 * np.exp(X_org))
      y = np.dot(X_org, w)
```

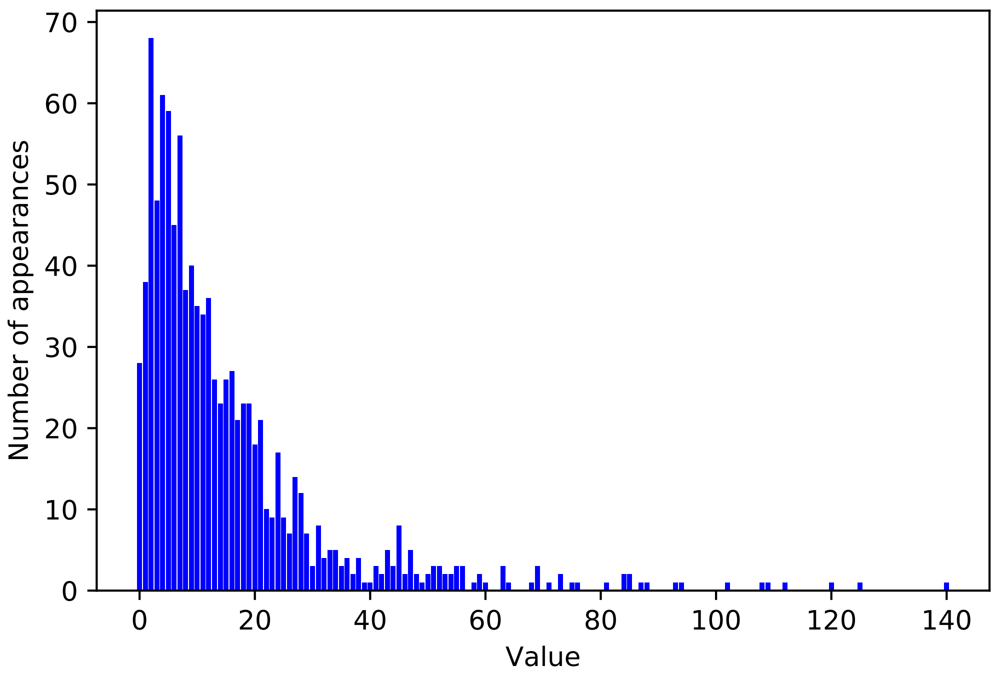
```
[28]: print("Number of feature appearances:\n{}".format(np.bincount(X[:, 0])))
```

```
Number of feature appearances:
[28 38 68 48 61 59 45 56 37 40 35 34 36 26 23 26 27 21 23 23 18 21 10  9
 17  9  7 14 12  7  3  8  4  5  5  3  4  2  4  1  1  3  2  5  3  8  2  5
  2  1  2  3  3  2  2  3  3  0  1  2  1  0  0  3  1  0  0  0  1  3  0  1
  0  2  0  1  1  0  0  0  0  1  0  0  2  2  0  1  1  0  0  0  0  1  1  0
  0  0  0  0  0  0  1  0  0  0  0  0  1  1  0  0  1  0  0  0  0  0  0  0
  1  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1]
```

```
[29]: bins = np.bincount(X[:, 0])
      plt.bar(range(len(bins)), bins, color='b')
```

```
plt.ylabel("Number of appearances")
plt.xlabel("Value")
```

```
<matplotlib.text.Text at 0x116441400>
```



This is something most linear models can't handle very well:

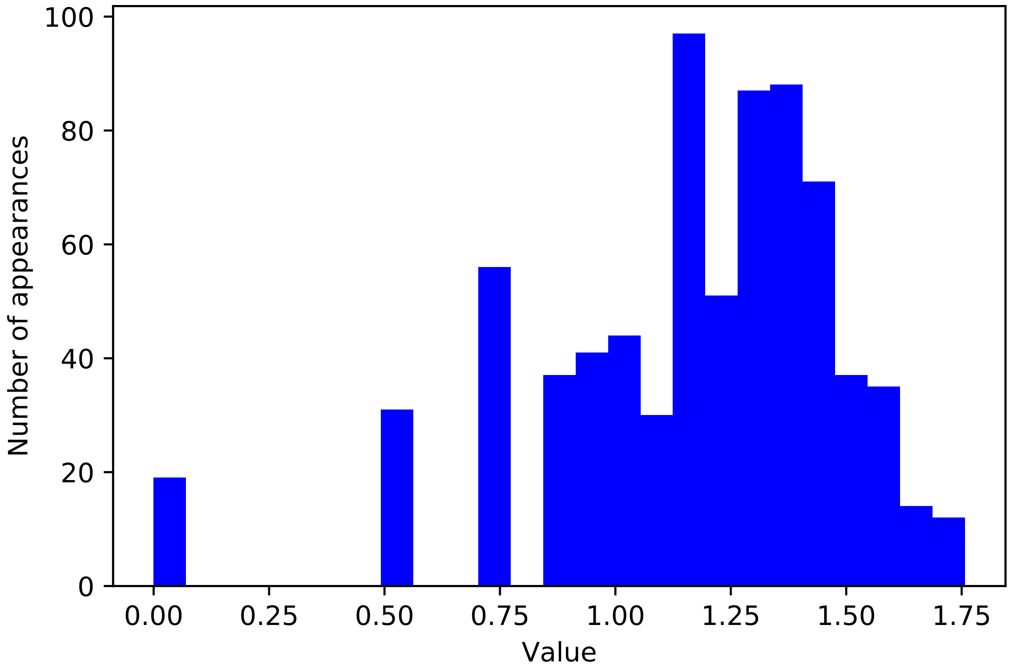
```
[30]: from sklearn.linear_model import Ridge
      X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
      score = Ridge().fit(X_train, y_train).score(X_test, y_test)
      print("Test score: {:.3f}".format(score))
```

```
Test score: 0.622
```

Applying a logarithmic transformation can help to create a more normal (Gaussian) distribution

```
[31]: # We actually compute log(x+1) to avoid the occurrence of log(0)
      X_train_log = np.log(X_train + 1)
      X_test_log = np.log(X_test + 1)
```

```
[32]: plt.hist(np.log(X_train_log[:, 0] + 1), bins=25, color='b')
      plt.ylabel("Number of appearances")
      plt.xlabel("Value");
```



And our Ridge regressor now performs a lot better.

```
[33]: score = Ridge().fit(X_train_log, y_train).score(X_test_log, y_test)
      print("Test score: {:.3f}".format(score))
```

```
Test score: 0.875
```

Finding the transformation that works best for each combination of dataset and model is somewhat of an art.

Automatic Feature Selection

When adding new features, or with high-dimensional datasets in general, it can be a good idea to reduce the number of features to only the most useful ones, and discard the rest. - Simpler models that generalize better - Help algorithms that are sensitive to the number of features (e.g. kNN).

Univariate statistics (ANOVA) We want to keep the features for which there is statistically significant relationship between it and the target. In the case of classification, this is also known as analysis of variance (ANOVA). These test consider each feature individually (they are univariate), and are completely independent of the model that you might want to apply afterwards. The result will be a p-value for each feature (lower is better).

In scikit-learn": - `SelectKBest` will only keep the k features with the lowest p values. - `SelectPercentile` selects a fixed percentage of features.

To test these methods, we'll take the `breast_cancer` dataset, and add 50 random noise features. The feature selector should be able to remove at least these noise features.

```
[34]: from sklearn.datasets import load_breast_cancer
      from sklearn.feature_selection import SelectPercentile
```

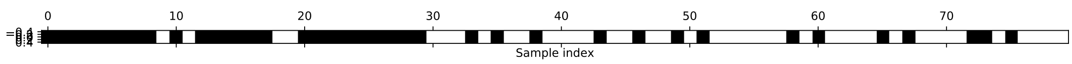
```
from sklearn.model_selection import train_test_split

cancer = load_breast_cancer()

# get deterministic random numbers
rng = np.random.RandomState(42)
noise = rng.normal(size=(len(cancer.data), 50))
# add noise features to the data
# the first 30 features are from the dataset, the next 50 are noise
X_w_noise = np.hstack([cancer.data, noise])

X_train, X_test, y_train, y_test = train_test_split(
    X_w_noise, cancer.target, random_state=0, test_size=.5)
# use f_classif (the default) and SelectPercentile to select 50% of featur
select = SelectPercentile(percentile=50)
select.fit(X_train, y_train)
# transform training set:
X_train_selected = select.transform(X_train)

print("X_train.shape: {}".format(X_train.shape))
print("X_train_selected.shape: {}".format(X_train_selected.shape))
```

```
X_train.shape: (284, 80)
X_train_selected.shape: (284, 40)
```

We can retrieve which features were selected with `get_support`, and visualize the selected (black) and removed (white) features. `SelectPercentile` removed most of the noise features, but not perfectly.

```
[35]: mask = select.get_support()
      # visualize the mask. black is True, white is False
      plt.matshow(mask.reshape(1, -1), cmap='gray_r')
      plt.xlabel("Sample index")
```

```
<matplotlib.text.Text at 0x11f07cb00>
```



As usual, we need to check how the transformation affects the performance of our learning algorithms.

```
[36]: from sklearn.linear_model import LogisticRegression

      # transform test data:
      X_test_selected = select.transform(X_test)

      lr = LogisticRegression()
      lr.fit(X_train, y_train)
```

```
print("Score with all features: {:.3f}".format(lr.score(X_test, y_test)))
lr.fit(X_train_selected, y_train)
print("Score with only selected features: {:.3f}".format(
        lr.score(X_test_selected, y_test)))
```

```
Score with all features: 0.930
Score with only selected features: 0.940
```

Model-based Feature Selection Model-based feature selection uses a supervised machine learning model to judge the importance of each feature, and keeps only the most important ones. Compared to ANOVA, they consider all features together, and are thus able to capture interactions: a feature may be more (or less) informative in combination with others.

The supervised model that is used for feature selection doesn't need to be the same model that is used for the final supervised modeling, it only needs to be able to measure the (perceived) importance for each feature:

- Decision tree–based models return a `feature_importances_` attribute
- Linear models return coefficients, whose absolute values also reflect feature importance

In scikit-learn, we can do this using `SelectFromModel`. It requires a model and a threshold. Threshold='median' means that the median observed feature importance will be the threshold, which will remove 50% of the features.

We've seen before how RandomForests return good estimates of feature importance:

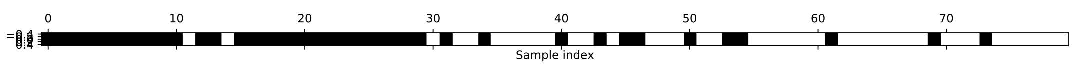
```
[37]: from sklearn.feature_selection import SelectFromModel
      from sklearn.ensemble import RandomForestClassifier
      select = SelectFromModel(
          RandomForestClassifier(n_estimators=100, random_state=42),
          threshold="median")
```

```
[38]: select.fit(X_train, y_train)
      X_train_l1 = select.transform(X_train)
      print("X_train.shape: {}".format(X_train.shape))
      print("X_train_l1.shape: {}".format(X_train_l1.shape))
```

```
X_train.shape: (284, 80)
X_train_l1.shape: (284, 40)
```

```
[39]: mask = select.get_support()
      # visualize the mask. black is True, white is False
      plt.matshow(mask.reshape(1, -1), cmap='gray_r')
      plt.xlabel("Sample index")
```

```
<matplotlib.text.Text at 0x11f0dc5c0>
```



All but two of the original features were selected, and most of the noise features removed. Our linear model trained on the selected features also performs quite a bit better.

```
[40]: X_test_l1 = select.transform(X_test)
      score = LogisticRegression().fit(X_train_l1, y_train).score(X_test_l1, y_t
      print("Test score: {:.3f}".format(score))
```

```
Test score: 0.951
```

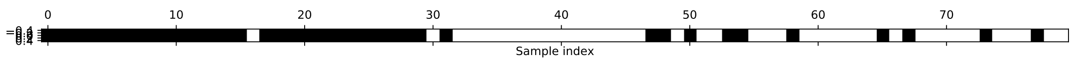
Iterative feature selection Instead of building a model to remove many features at once, we can also just ask it to remove the worst feature, then retrain, remove another feature, etc. This is known as *recursive feature elimination* (RFE).

Vice versa, we couls also ask it to iteratively add one feature at a time. This is called *forward selection*.

In both cases, we need to define beforehand how many features to select. When this is unknown, one often considers this as an additional hyperparameter of the whole process (pipeline) that needs to be optimized.

```
[41]: from sklearn.feature_selection import RFE
      select = RFE(RandomForestClassifier(n_estimators=100, random_state=42),
                   n_features_to_select=40)

      select.fit(X_train, y_train)
      # visualize the selected features:
      mask = select.get_support()
      plt.matshow(mask.reshape(1, -1), cmap='gray_r')
      plt.xlabel("Sample index")
```

```
<matplotlib.text.Text at 0x11fb1e320>
```




```
[42]: X_train_rfe = select.transform(X_train)
      X_test_rfe = select.transform(X_test)

      score = LogisticRegression().fit(X_train_rfe, y_train).score(X_test_rfe, y
      print("Test score: {:.3f}".format(score))
```

```
Test score: 0.951
```

```
[43]: print("Test score: {:.3f}".format(select.score(X_test, y_test)))
```

```
Test score: 0.951
```

Automatic feature selection can be helpful when:

- You expect some inputs to be uninformative, and your model does not select features internally (as tree-based models do)
- You need to speed up prediction without loosing much accuracy
- You want a more interpretable model (with fewer variables)

Scaling

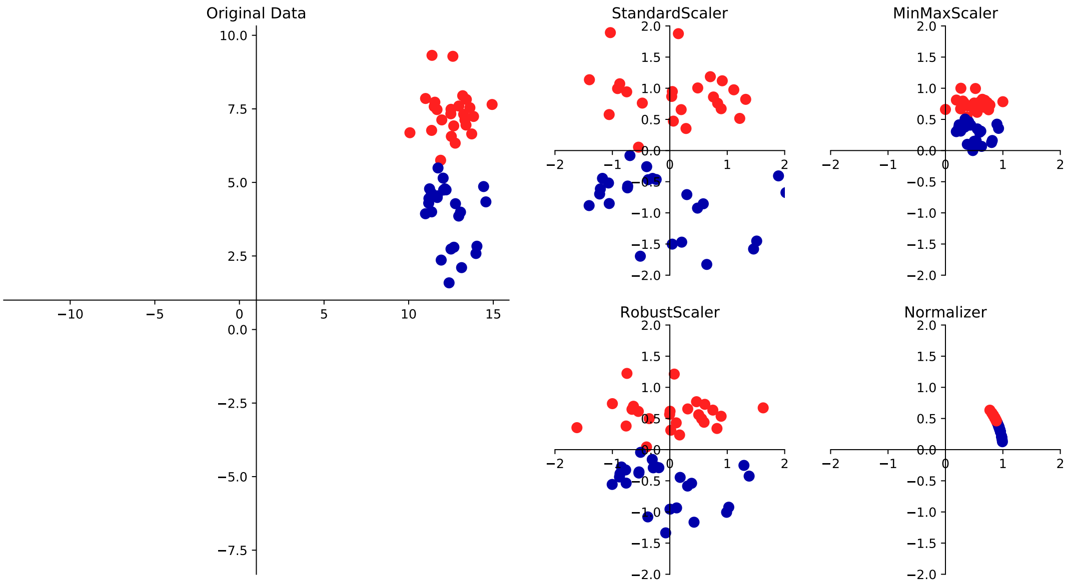
When the features have different scales (their values range between very different minimum and maximum values), it makes sense to scale them to the same range. Otherwise, one feature will overpower the others, expecially when raised to the nth power.

- We can rescale features between 0 and 1 using MinMaxScaler.
- Remember to `fit_transform` the training data, then `transform` the test data

[44]:
```
from sklearn.datasets import load_boston
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

boston = load_boston()
X_train, X_test, y_train, y_test = train_test_split(boston.data, boston.ta
                                                     random_state=0)

# rescale data:
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

Several scaling techniques are available: - `StandardScaler` rescales all features to mean=0 and variance=1 - Does not ensure and min/max value - `RobustScaler` uses the median and quartiles - Median m: half of the values < m, half > m - Lower Quartile lq: 1/4 of values < lq - Upper Quartile uq: 1/4 of values > uq - Ignores *outliers*, brings all features to same scale - `MinMaxScaler` brings all feature values between 0 and 1 - `Normalizer` scales data such that the feature vector has Euclidean length 1 - Projects data to the unit circle - Used when only the direction/angle of the data matters

[45]:
```
mglearn.plots.plot_scaling()
```



Applying scaling transformations

- Lets apply a scaling transformation *manually*, then use it to train a learning algorithm
- First, split the data in training and test set

```
[46]: from sklearn.datasets import load_breast_cancer
      from sklearn.model_selection import train_test_split
      cancer = load_breast_cancer()

      X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.ta
                                                          random_state=1)
```

- Next, we `fit` the preprocessor on the **training data**
  - This computes the necessary transformation parameters
  - For `MinMaxScaler`, these are the min/max values for every feature

```
[47]: from sklearn.preprocessing import MinMaxScaler

      scaler = MinMaxScaler()
      scaler.fit(X_train)
```

```
MinMaxScaler(copy=True, feature_range=(0, 1))
```

- After fitting, we can `transform` the training and test data

```
[48]: # transform training data
      X_train_scaled = scaler.transform(X_train)
      # print dataset properties before and after scaling
      print("per-feature minimum before scaling:\n {}".format(X_train.min(axis=0
      print("per-feature maximum before scaling:\n {}".format(X_train.max(axis=0
      print("per-feature minimum after scaling:\n {}".format(
                X_train_scaled.min(axis=0)))
      print("per-feature maximum after scaling:\n {}".format(
                X_train_scaled.max(axis=0)))
```

```
per-feature minimum before scaling:
 [   6.981    9.71    43.79   143.5      0.053    0.019    0.       0.       0.106
    0.05     0.115    0.36     0.757    6.802    0.002    0.002    0.       0.
    0.01     0.001    7.93    12.02    50.41   185.2      0.071    0.027    0.
    0.       0.157    0.055]
per-feature maximum before scaling:
 [  28.11     39.28    188.5    2501.        0.163     0.287     0.427     0.201
     0.304     0.096     2.873     4.885    21.98    542.2       0.031     0.135
     0.396     0.053     0.061     0.03     36.04     49.54    251.2    4254.
     0.223     0.938     1.17      0.291     0.577     0.149]
per-feature minimum after scaling:
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
 0. 0. 0. 0. 0. 0.]
per-feature maximum after scaling:
 [1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1.]
```

```
[49]: # transform test data
      X_test_scaled = scaler.transform(X_test)
      # print test data properties after scaling
      print("per-feature minimum after scaling:\n{}".format(X_test_scaled.min(ax
      print("per-feature maximum after scaling:\n{}".format(X_test_scaled.max(ax
```

```
per-feature minimum after scaling:
[ 0.034  0.023  0.031  0.011  0.141  0.044  0.     0.     0.154 -0.006
 -0.001  0.006  0.004  0.001  0.039  0.011  0.     0.    -0.032  0.007
  0.027  0.058  0.02   0.009  0.109  0.026  0.     0.    -0.    -0.002]
per-feature maximum after scaling:
[0.958 0.815 0.956 0.894 0.811 1.22  0.88  0.933 0.932 1.037 0.427 0.498
 0.441 0.284 0.487 0.739 0.767 0.629 1.337 0.391 0.896 0.793 0.849 0.745
 0.915 1.132 1.07  0.924 1.205 1.631]
```

- After scaling the test data, the values are not exactly between 0 and 1
- This is correct: we used the min/max values from the training data only
- We are still interested in how well our preprocessing+learning model generalizes from the training to the test data

- Remember to `fit` and `transform` on the training data, then `transform` the test data

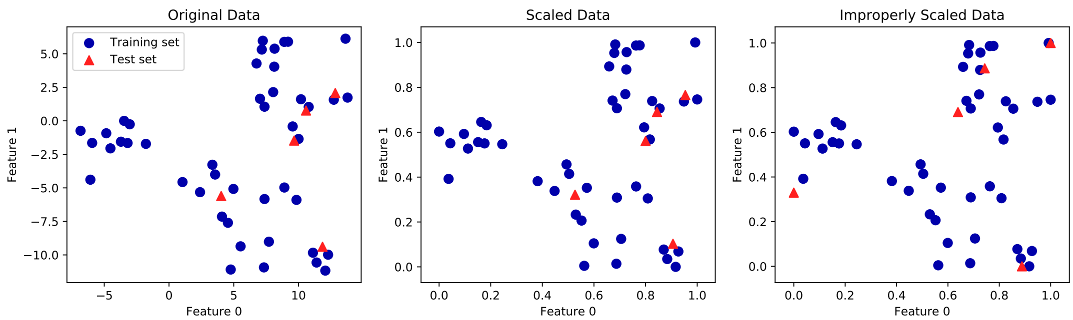
- 2nd figure: `fit` on training set, `transform` on training and test set

- 3rd figure: `fit` and `transform` on the training data

  - Test data points nowhere near same training data points
  - Trained model will have a hard time generalizing correctly

```
[50]: from sklearn.datasets import make_blobs
      # make synthetic data
      X, _ = make_blobs(n_samples=50, centers=5, random_state=4, cluster_std=2)
      # split it into training and test set
      X_train, X_test = train_test_split(X, random_state=5, test_size=.1)

      # plot the training and test set
      fig, axes = plt.subplots(1, 3, figsize=(13, 4))
      axes[0].scatter(X_train[:, 0], X_train[:, 1],
                      c=mglearn.cm2(0), label="Training set", s=60)
      axes[0].scatter(X_test[:, 0], X_test[:, 1], marker='^',
                      c=mglearn.cm2(1), label="Test set", s=60)
      axes[0].legend(loc='upper left')
      axes[0].set_title("Original Data")

      # scale the data using MinMaxScaler
      scaler = MinMaxScaler()
      scaler.fit(X_train)
      X_train_scaled = scaler.transform(X_train)
      X_test_scaled = scaler.transform(X_test)

      # visualize the properly scaled data
      axes[1].scatter(X_train_scaled[:, 0], X_train_scaled[:, 1],
```

```
                c=mglearn.cm2(0), label="Training set", s=60)
axes[1].scatter(X_test_scaled[:, 0], X_test_scaled[:, 1], marker='^',
                c=mglearn.cm2(1), label="Test set", s=60)
axes[1].set_title("Scaled Data")

# rescale the test set separately
# so that test set min is 0 and test set max is 1
# DO NOT DO THIS! For illustration purposes only
test_scaler = MinMaxScaler()
test_scaler.fit(X_test)
X_test_scaled_badly = test_scaler.transform(X_test)

# visualize wrongly scaled data
axes[2].scatter(X_train_scaled[:, 0], X_train_scaled[:, 1],
                c=mglearn.cm2(0), label="training set", s=60)
axes[2].scatter(X_test_scaled_badly[:, 0], X_test_scaled_badly[:, 1],
                marker='^', c=mglearn.cm2(1), label="test set", s=60)
axes[2].set_title("Improperly Scaled Data")

for ax in axes:
    ax.set_xlabel("Feature 0")
    ax.set_ylabel("Feature 1")
fig.tight_layout()
```



- Note: you can fit and transform the training together with `fit_transform`
- To transform the test data, you always need to `fit` on the training data and `transform` the test data

[51]:
```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
# calling fit and transform in sequence (using method chaining)
X_scaled = scaler.fit(X).transform(X)
# same result, but more efficient computation
X_scaled_d = scaler.fit_transform(X)
```

How great is the effect of scaling?

- First, we train the (linear) SVM without scaling

```
[52]: from sklearn.svm import LinearSVC

      X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.ta
                                                          random_state=0)

      svm = LinearSVC()
      svm.fit(X_train, y_train)
      print("Test set accuracy: {:.2f}".format(svm.score(X_test, y_test)))
```

```
Test set accuracy: 0.92
```

- With scaling, we get a much better model

```
[53]: # preprocessing using 0-1 scaling
      scaler = MinMaxScaler()
      scaler.fit(X_train)
      X_train_scaled = scaler.transform(X_train)
      X_test_scaled = scaler.transform(X_test)

      # learning an SVM on the scaled training data
      svm.fit(X_train_scaled, y_train)
      # scoring on the scaled test set
      print("Scaled test set accuracy: {:.2f}".format(svm.score(X_test_scaled, y
```

```
Scaled test set accuracy: 0.97
```

Scaling for polynomial regression

After scaling, we extract polynomial features and interactions up to a degree of 2. Note how we `fit` the `PolynomialFeatures` only on the training data and then apply it (`transform`) on both the training and test data.

`PolynomialFeatures` will add a new features for each possible interaction (product) of up to 2 input features, including the products of a feature with itself (the squares). Hence, $\frac{13!}{11!2!}$ + 13 + 13 features total.

```
[54]: from sklearn.datasets import load_boston
      from sklearn.model_selection import train_test_split
      from sklearn.preprocessing import MinMaxScaler

      boston = load_boston()
      X_train, X_test, y_train, y_test = train_test_split(boston.data, boston.ta
                                                          random_state=0)

      # rescale data:
      scaler = MinMaxScaler()
      X_train_scaled = scaler.fit_transform(X_train)
      X_test_scaled = scaler.transform(X_test)
```

```
[55]: poly = PolynomialFeatures(degree=2).fit(X_train_scaled)
      X_train_poly = poly.transform(X_train_scaled)
      X_test_poly = poly.transform(X_test_scaled)
```

```
print("X_train.shape: {}".format(X_train.shape))
print("X_train_poly.shape: {}".format(X_train_poly.shape))
```

```
X_train.shape: (379, 13)
X_train_poly.shape: (379, 105)
```

The exact correspondence between input and output features can be found using the get_feature_names method:

```
[56]: print("Polynomial feature names:\n{}".format(poly.get_feature_names()))
```

```
Polynomial feature names:
['1', 'x0', 'x1', 'x2', 'x3', 'x4', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10', 'x11',
```

Let's compare the performance of a linear model (Ridge regression) on the data with and without interactions:

```
[57]: from sklearn.linear_model import Ridge
      ridge = Ridge().fit(X_train_scaled, y_train)
      print("Score without interactions: {:.3f}".format(
              ridge.score(X_test_scaled, y_test)))
      ridge = Ridge().fit(X_train_poly, y_train)
      print("Score with interactions: {:.3f}".format(
              ridge.score(X_test_poly, y_test)))
```

```
Score without interactions: 0.621
Score with interactions: 0.753
```

Clearly, the interactions and polynomial features gave us a good boost in performance when using Ridge. When using a more complex model like a random forest, the story is a bit different, though:

```
[58]: from sklearn.ensemble import RandomForestRegressor
      rf = RandomForestRegressor(n_estimators=100).fit(X_train_scaled, y_train)
      print("Score without interactions: {:.3f}".format(
              rf.score(X_test_scaled, y_test)))
      rf = RandomForestRegressor(n_estimators=100).fit(X_train_poly, y_train)
      print("Score with interactions: {:.3f}".format(rf.score(X_test_poly, y_tes
```

```
Score without interactions: 0.795
Score with interactions: 0.767
```

The random forest does not benefit from the interaction features, in fact, performance decreases...

Adding polynomials is typically good for linear models, but not a cure-for-all. Always evaluate the performance of models when adding preprocessing steps.

- What if we want the cross-validated evaluation?
  - Apply scaling on every fold independently?

Building Pipelines

- In scikit-learn, a `pipeline` combines multiple processing *steps* in a single estimator
- All but the last step should be transformer (have a `transform` method)
  - The last step can be a transformer too (e.g. Scaler+PCA)
- It has a `fit`, `predict`, and `score` method, just like any other learning algorithm
- Pipelines are built as a list of steps, which are (name, algorithm) tuples
  - The name can be anything you want, but can't contain `'__'`
  - We use `'__'` to refer to the hyperparameters, e.g. `svm__C`
- Let's build, train, and score a `MinMaxScaler` + `LinearSVC` pipeline:

```
[61]: from sklearn.pipeline import Pipeline
      pipe = Pipeline([("scaler", MinMaxScaler()), ("svm", LinearSVC())])

      X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.ta
                                                          random_state=1)
      pipe.fit(X_train, y_train)
      print("Test score: {:.2f}".format(pipe.score(X_test, y_test)))
```

```
Test score: 0.97
```

- Now with cross-validation:

```
[62]: from sklearn.model_selection import cross_val_score
      scores = cross_val_score(pipe, cancer.data, cancer.target)
      print("Cross-validation scores: {}".format(scores))
      print("Average cross-validation score: {:.2f}".format(scores.mean()))
```

```
Cross-validation scores: [0.984 0.953 0.979]
Average cross-validation score: 0.97
```

- We can retrieve the trained SVM by querying the right step indices

```
[63]: pipe.fit(X_train, y_train)
      print("SVM component: {}".format(pipe.steps[1][1]))
```

```
SVM component: LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
     verbose=0)
```

- Or we can use the `named_steps` dictionary

```
[64]: print("SVM component: {}".format(pipe.named_steps['svm']))
```

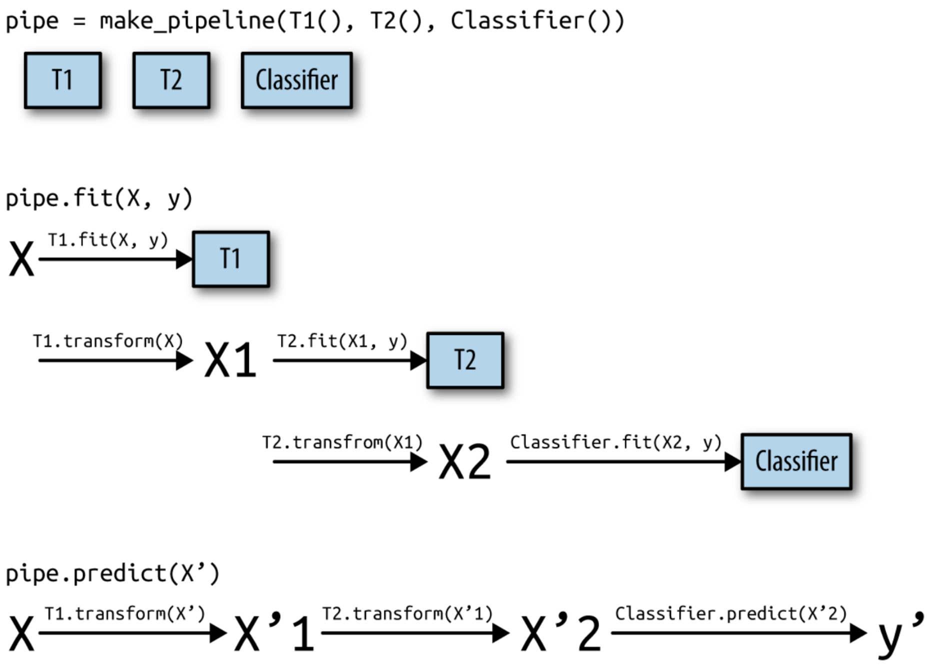
```
SVM component: LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
     verbose=0)
```

- When you don't need specific names for specific steps, you can use make_pipeline
  - Assigns names to steps automatically

```
[65]: from sklearn.pipeline import make_pipeline
      # standard syntax
      pipe_long = Pipeline([("scaler", MinMaxScaler()), ("svm", LinearSVC(C=100)
      # abbreviated syntax
      pipe_short = make_pipeline(MinMaxScaler(), LinearSVC(C=100))
      print("Pipeline steps:\n{}".format(pipe_short.steps))
```

```
Pipeline steps:
[('minmaxscaler', MinMaxScaler(copy=True, feature_range=(0, 1))), ('linearsvc',
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
     verbose=0))]
```

Visualization of a pipeline fit and predict



pipeline_illustration