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5.3. Preprocessing data

The sklearn.preprocessing package provides several common utility functions and transformer classes to change raw feature vectors into a representation that is more suitable for the downstream estimators.

In general, learning algorithms benefit from standardization of the data set. If some outliers are present in the set, robust scalers or transformers are more appropriate. The behaviors of the different scalers, transformers, and normalizers on a dataset containing marginal outliers is highlighted in Compare the effect of different scalers on data with outliers.

5.3.1. Standardization, or mean removal and variance scaling

Standardization of datasets is a **common requirement for many machine learning estimators** implemented in scikit-learn; they might behave badly if the individual features do not more or less look like standard normally distributed data: Gaussian with **zero mean and unit variance**.

In practice we often ignore the shape of the distribution and just transform the data to center it by removing the mean value of each feature, then scale it by dividing non-constant features by their standard deviation.

For instance, many elements used in the objective function of a learning algorithm (such as the RBF kernel of Support Vector Machines or the I1 and I2 regularizers of linear models) assume that all features are centered around zero and have variance in the same order. If a feature has a variance that is orders of magnitude larger than others, it might dominate the objective function and make the estimator unable to learn from other features correctly as expected.

The function **scale** provides a quick and easy way to perform this operation on a single array-like dataset:

Scaled data has zero mean and unit variance:

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```
>>> X_scaled.mean(axis=0)
array([0., 0., 0.])
>>> X_scaled.std(axis=0)
array([1., 1., 1.])
```

The preprocessing module further provides a utility class **StandardScaler** that implements the Transformer API to compute the mean and standard deviation on a training set so as to be able to later reapply the same transformation on the testing set. This class is hence suitable for use in the early steps of a **sklearn.pipeline.Pipeline**:

The scaler instance can then be used on new data to transform it the same way it did on the training set:

```
>>> X_test = [[-1., 1., 0.]]
>>> scaler.transform(X_test)
array([[-2.44..., 1.22..., -0.26...]])
```

It is possible to disable either centering or scaling by either passing with_mean=False or with_std=False to the constructor of **StandardScaler**.

5.3.1.1. Scaling features to a range

An alternative standardization is scaling features to lie between a given minimum and maximum value, often between zero and one, or so that the maximum absolute value of each feature is scaled to unit size. This can be achieved using MinMaxScaler or MaxAbsScaler, respectively.

The motivation to use this scaling include robustness to very small standard deviations of features and preserving zero entries in sparse data.

Here is an example to scale a toy data matrix to the [0, 1] range:

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The same instance of the transformer can then be applied to some new test data unseen during the fit call: the same scaling and shifting operations will be applied to be consistent with the transformation performed on the train data:

It is possible to introspect the scaler attributes to find about the exact nature of the transformation learned on the training data:

If MinMaxScaler is given an explicit feature range=(min, max) the full formula is:

```
X_std = (X - X.min(axis=0)) / (X.max(axis=0) - X.min(axis=0))

X_scaled = X_std * (max - min) + min
```

MaxAbsScaler works in a very similar fashion, but scales in a way that the training data lies within the range [-1, 1] by dividing through the largest maximum value in each feature. It is meant for data that is already centered at zero or sparse data.

Here is how to use the toy data from the previous example with this scaler:

As with **scale**, the module further provides convenience functions **minmax_scale** and **maxabs scale** if you don't want to create an object.

5.3.1.2. Scaling sparse data

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Centering sparse data would destroy the sparseness structure in the data, and thus rarely is a sensible thing to do. However, it can make sense to scale sparse inputs, especially if features are on different scales.

MaxAbsScaler and maxabs_scale were specifically designed for scaling sparse data, and are the recommended way to go about this. However, scale and StandardScaler can accept scipy.sparse matrices as input, as long as with_mean=False is explicitly passed to the constructor. Otherwise a ValueError will be raised as silently centering would break the sparsity and would often crash the execution by allocating excessive amounts of memory unintentionally.

RobustScaler cannot be fitted to sparse inputs, but you can use the transform method on sparse inputs.

Note that the scalers accept both Compressed Sparse Rows and Compressed Sparse Columns format (see scipy.sparse.csr_matrix and scipy.sparse.csc_matrix). Any other sparse input will be **converted to the Compressed Sparse Rows representation**. To avoid unnecessary memory copies, it is recommended to choose the CSR or CSC representation upstream.

Finally, if the centered data is expected to be small enough, explicitly converting the input to an array using the toarray method of sparse matrices is another option.

5.3.1.3. Scaling data with outliers

If your data contains many outliers, scaling using the mean and variance of the data is likely to not work very well. In these cases, you can use **robust_scale** and **RobustScaler** as drop-in replacements instead. They use more robust estimates for the center and range of your data.

PrevReferences:

Further discussion on the importance of centering and scaling data is available on this FAQ: Should I normalize/standardize/rescale the data?

Scaling vs Whitening

It is sometimes not enough to center and scale the features independently, since a downstream model can further make some assumption on the linear independence of the features.

To address this issue you can use **sklearn.decomposition.PCA** with whiten=True to further remove the linear correlation across features.

Scaling a 1D array

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All above functions (i.e. **scale**, **minmax_scale**, **maxabs_scale**, and **robust_scale**) accept 1D array which can be useful in some specific case.

5.3.1.4. Centering kernel matrices

If you have a kernel matrix of a kernel K that computes a dot product in a feature space defined by function phi, a **KernelCenterer** can transform the kernel matrix so that it contains inner products in the feature space defined by phi followed by removal of the mean in that space.

5.3.2. Non-linear transformation

Two types of transformations are available: quantile transforms and power transforms. Both quantile and power transforms are based on monotonic transformations of the features and thus preserve the rank of the values along each feature.

Quantile transforms put all features into the same desired distribution based on the formula $G^{-1}(F(X))$ where F is the cumulative distribution function of the feature and G^{-1} the quantile function of the desired output distribution G. This formula is using the two following facts: (i) if X is a random variable with a continuous cumulative distribution function F then F(X) is uniformly distributed on [0,1]; (ii) if U is a random variable with uniform distribution on [0,1] then $G^{-1}(U)$ has distribution G. By performing a rank transformation, a quantile transform smooths out unusual distributions and is less influenced by outliers than scaling methods. It does, however, distort correlations and distances within and across features.

Power transforms are a family of parametric transformations that aim to map data from any distribution to as close to a Gaussian distribution.

5.3.2.1. Mapping to a Uniform distribution

QuantileTransformer and **quantile_transform** provide a non-parametric transformation to map the data to a uniform distribution with values between 0 and 1:

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.model_selection import train_test_split
>>> iris = load_iris()
>>> X, y = iris.data, iris.target
>>> X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
>>> quantile_transformer = preprocessing.QuantileTransformer(random_state=0)
>>> X_train_trans = quantile_transformer.fit_transform(X_train)
>>> X_test_trans = quantile_transformer.transform(X_test)
>>> np.percentile(X_train[:, 0], [0, 25, 50, 75, 100])
array([ 4.3, 5.1, 5.8, 6.5, 7.9])
```

This feature corresponds to the sepal length in cm. Once the quantile transformation applied, those landmarks approach closely the percentiles previously defined:

```
>>> np.percentile(X_train_trans[:, 0], [0, 25, 50, 75, 100])
...
array([ 0.00..., 0.24..., 0.49..., 0.73..., 0.99...])
```

This can be confirmed on a independent testing set with similar remarks:

```
>>> np.percentile(X_test[:, 0], [0, 25, 50, 75, 100])
...
array([ 4.4 , 5.125, 5.75 , 6.175, 7.3 ])
>>> np.percentile(X_test_trans[:, 0], [0, 25, 50, 75, 100])
...
array([ 0.01..., 0.25..., 0.46..., 0.60... , 0.94...])
```

5.3.2.2. Mapping to a Gaussian distribution

In many modeling scenarios, normality of the features in a dataset is desirable. Power transforms are a family of parametric, monotonic transformations that aim to map data from any distribution to as close to a Gaussian distribution as possible in order to stabilize variance and minimize skewness.

PowerTransformer currently provides two such power transformations, the Yeo-Johnson transform and the Box-Cox transform.

The Yeo-Johnson transform is given by:

$$x_i^{(\lambda)} = egin{cases} [(x_i+1)^{\lambda}-1]/\lambda & ext{if } \lambda
eq 0, x_i \geq 0, \ \ln{(x_i)}+1 & ext{if } \lambda = 0, x_i \geq 0 \ -[(-x_i+1)^{2-\lambda}-1]/(2-\lambda) & ext{if } \lambda
eq 2, x_i < 0, \ -\ln{(-x_i+1)} & ext{if } \lambda = 2, x_i < 0 \end{cases}$$

while the Box-Cox transform is given by:

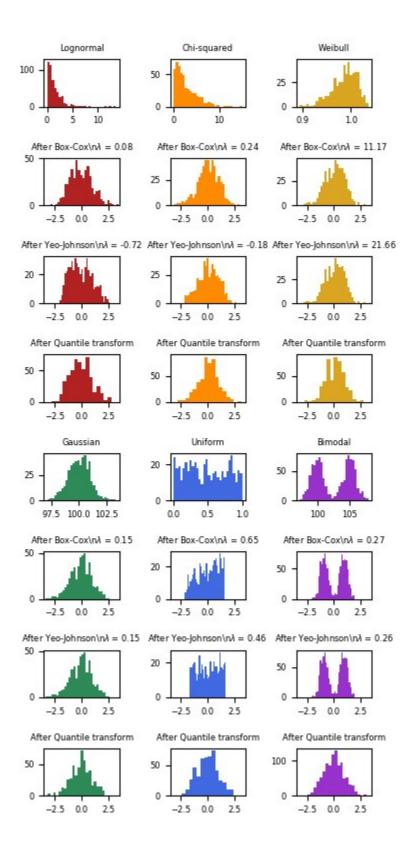
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$$x_i^{(\lambda)} = egin{cases} rac{x_i^{\lambda}-1}{\lambda} & ext{if } \lambda
eq 0, \ \ln{(x_i)} & ext{if } \lambda = 0, \end{cases}$$

Box-Cox can only be applied to strictly positive data. In both methods, the transformation is parameterized by λ , which is determined through maximum likelihood estimation. Here is an example of using Box-Cox to map samples drawn from a lognormal distribution to a normal distribution:

While the above example sets the standardize option to False, **PowerTransformer** will apply zero-mean, unit-variance normalization to the transformed output by default.

Below are examples of Box-Cox and Yeo-Johnson applied to various probability distributions. Note that when applied to certain distributions, the power transforms achieve very Gaussian-like results, but with others, they are ineffective. This highlights the importance of visualizing the data before and after transformation.



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It is also possible to map data to a normal distribution using **QuantileTransformer** by setting output_distribution='normal'. Using the earlier example with the iris dataset:

Thus the median of the input becomes the mean of the output, centered at 0. The normal output is clipped so that the input's minimum and maximum — corresponding to the 1e-7 and 1 - 1e-7 quantiles respectively — do not become infinite under the transformation.

5.3.3. Normalization

Normalization is the process of **scaling individual samples to have unit norm**. This process can be useful if you plan to use a quadratic form such as the dot-product or any other kernel to quantify the similarity of any pair of samples.

This assumption is the base of the Vector Space Model often used in text classification and clustering contexts.

The function **normalize** provides a quick and easy way to perform this operation on a single array-like dataset, either using the 11 or 12 norms:

The preprocessing module further provides a utility class **Normalizer** that implements the same operation using the Transformer API (even though the fit method is useless in this case: the class is stateless as this operation treats samples independently).

This class is hence suitable for use in the early steps of a **sklearn.pipeline.Pipeline**:

```
>>> normalizer = preprocessing.Normalizer().fit(X) # fit does nothing
>>> normalizer
Normalizer(copy=True, norm='12')
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The normalizer instance can then be used on sample vectors as any transformer:

```
>>> normalizer.transform(X)
array([[ 0.40..., -0.40...,  0.81...],
       [ 1. ...,  0. ...,  0. ...],
       [ 0. ...,  0.70..., -0.70...]])

>>> normalizer.transform([[-1.,  1.,  0.]])
array([[-0.70...,  0.70...,  0. ...]])
```

Sparse input

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normalize and Normalizer accept both dense array-like and sparse matrices from scipy.sparse as input.

For sparse input the data is **converted to the Compressed Sparse Rows representation** (see scipy.sparse.csr_matrix) before being fed to efficient Cython routines. To avoid unnecessary memory copies, it is recommended to choose the CSR representation upstream.

5.3.4. Encoding categorical features

Often features are not given as continuous values but categorical. For example a person could have features ["male", "female"], ["from Europe", "from US", "from Asia"], ["uses Firefox", "uses Chrome", "uses Safari", "uses Internet Explorer"]. Such features can be efficiently coded as integers, for instance ["male", "from US", "uses Internet Explorer"] could be expressed as [0, 1, 3] while ["female", "from Asia", "uses Chrome"] would be [1, 2, 1].

To convert categorical features to such integer codes, we can use the **OrdinalEncoder**. This estimator transforms each categorical feature to one new feature of integers (0 to n categories - 1):

```
>>> enc = preprocessing.OrdinalEncoder()
>>> X = [['male', 'from US', 'uses Safari'], ['female', 'from Europe', 'uses Fi
>>> enc.fit(X)
OrdinalEncoder(categories='auto', dtype=<... 'numpy.float64'>)
>>> enc.transform([['female', 'from US', 'uses Safari']])
array([[0., 1., 1.]])
```

Such integer representation can, however, not be used directly with all scikit-learn estimators, as these expect continuous input, and would interpret the categories as being ordered, which is often not desired (i.e. the set of browsers was ordered arbitrarily).

Another possibility to convert categorical features to features that can be used with scikit-learn estimators is to use a one-of-K, also known as one-hot or dummy encoding. This type of encoding can Previous

be obtained with the **OneHotEncoder**, which transforms each categorical feature with n_categories possible values into n_categories binary features, with one of them 1, and all others 0.

Continuing the example above:

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By default, the values each feature can take is inferred automatically from the dataset and can be found in the categories attribute:

```
>>> enc.categories_
[array(['female', 'male'], dtype=object), array(['from Europe', 'from US'], dty
```

It is possible to specify this explicitly using the parameter categories. There are two genders, four possible continents and four web browsers in our dataset:

If there is a possibility that the training data might have missing categorical features, it can often be better to specify handle_unknown='ignore' instead of setting the categories manually as above. When handle_unknown='ignore' is specified and unknown categories are encountered during transform, no error will be raised but the resulting one-hot encoded columns for this feature will be all zeros (handle_unknown='ignore' is only supported for one-hot encoding):

It is also possible to encode each column into n_categories - 1 columns instead of n_categories columns by using the drop parameter. This parameter allows the user to specify a category for each feature to be dropped. This is useful to avoid co-linearity in the input matrix in some classifiers. Such functionality is useful, for example, when using non-regularized regression (LinearRegression), since co-linearity would cause the covariance matrix to be non-invertible. When this parameter is not None, handle unknown must be set to error:

See Loading features from dicts for categorical features that are represented as a dict, not as scalars.

5.3.5. Discretization

Discretization (otherwise known as quantization or binning) provides a way to partition continuous features into discrete values. Certain datasets with continuous features may benefit from discretization, because discretization can transform the dataset of continuous attributes to one with only nominal attributes.

One-hot encoded discretized features can make a model more expressive, while maintaining interpretability. For instance, pre-processing with a discretizer can introduce nonlinearity to linear models.

5.3.5.1. K-bins discretization

KBinsDiscretizer discretizes features into k bins:

```
>>> X = np.array([[ -3., 5., 15 ],
Previous [ 0., 6., 14 ],
Next
```

```
... [ 6., 3., 11 ]])
>>> est = preprocessing.KBinsDiscretizer(n_bins=[3, 2, 2], encode='ordinal').fi
```

By default the output is one-hot encoded into a sparse matrix (See Encoding categorical features) and this can be configured with the encode parameter. For each feature, the bin edges are computed during fit and together with the number of bins, they will define the intervals. Therefore, for the current example, these intervals are defined as:

```
• feature 1: [-\infty, -1), [-1, 2), [2, \infty)
• feature 2: [-\infty, 5), [5, \infty)
• feature 3: [-\infty, 14), [14, \infty)
```

Based on these bin intervals, X is transformed as follows:

The resulting dataset contains ordinal attributes which can be further used in a **sklearn.pipeline.Pipeline**.

Discretization is similar to constructing histograms for continuous data. However, histograms focus on counting features which fall into particular bins, whereas discretization focuses on assigning feature values to these bins.

KBinsDiscretizer implements different binning strategies, which can be selected with the strategy parameter. The 'uniform' strategy uses constant-width bins. The 'quantile' strategy uses the quantiles values to have equally populated bins in each feature. The 'kmeans' strategy defines bins based on a k-means clustering procedure performed on each feature independently.

Examples:

- Using KBinsDiscretizer to discretize continuous features
- Feature discretization
- · Demonstrating the different strategies of KBinsDiscretizer

5.3.5.2. Feature binarization

Feature binarization is the process of thresholding numerical features to get boolean values.

This can be useful for downstream probabilistic estimators that make assumption that the input data is distributed according to a multi-variate Bernoulli distribution. For instance, this is the case for the sklearn.neural_network.BernoulliRBM.

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It is also common among the text processing community to use binary feature values (probably to simplify the probabilistic reasoning) even if normalized counts (a.k.a. term frequencies) or TF-IDF valued features often perform slightly better in practice.

As for the **Normalizer**, the utility class **Binarizer** is meant to be used in the early stages of **sklearn.pipeline.Pipeline**. The fit method does nothing as each sample is treated independently of others:

It is possible to adjust the threshold of the binarizer:

As for the **StandardScaler** and **Normalizer** classes, the preprocessing module provides a companion function **binarize** to be used when the transformer API is not necessary.

Note that the **Binarizer** is similar to the **KBinsDiscretizer** when k = 2, and when the bin edge is at the value threshold.

Sparse input

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binarize and **Binarizer** accept **both dense array-like and sparse matrices from scipy.sparse as input**.

For sparse input the data is **converted to the Compressed Sparse Rows representation** (see scipy.sparse.csr_matrix). To avoid unnecessary memory copies, it is recommended to choose the CSR representation upstream.

5.3.6. Imputation of missing values

Tools for imputing missing values are discussed at Imputation of missing values.

5.3.7. Generating polynomial features

Often it's useful to add complexity to the model by considering nonlinear features of the input data.

A simple and common method to use is polynomial features, which can get features' high-order and interaction terms. It is implemented in **PolynomialFeatures**:

The features of X have been transformed from (X_1,X_2) to $(1,X_1,X_2,X_1^2,X_1X_2,X_2^2)$.

In some cases, only interaction terms among features are required, and it can be gotten with the setting interaction only=True:

```
>>>
X = \text{np.arange}(9).\text{reshape}(3, 3)
>>> X
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]])
>>> poly = PolynomialFeatures(degree=3, interaction only=True)
>>> poly.fit transform(X)
array([[ 1.,
                0.,
                      1.,
                                 0.,
                                               2.,
                                                     0.1,
                            2.,
                                       0.,
                                 12., 15., 20., 60.],
          1.,
                3.,
                      4.,
                            5.,
                6.,
                                 42., 48., 56., 336.]])
         1.,
                      7.,
                            8.,
```

The features of X have been transformed from (X_1,X_2,X_3) to $(1,X_1,X_2,X_3,X_1X_2,X_1X_3,X_2X_3,X_1X_2X_3)$.

Note that polynomial features are used implicitly in kernel methods (e.g., **sklearn.svm.SVC**, **sklearn.decomposition.KernelPCA**) when using polynomial Kernel functions.

5.3.8. Custom transformers

pipeline, do:

Often, you will want to convert an existing Python function into a transformer to assist in data cleaning or processing. You can implement a transformer from an arbitrary function with **FunctionTransformer**. For example, to build a transformer that applies a log transformation in a

You can ensure that func and inverse_func are the inverse of each other by setting check_inverse=True and calling fit before transform. Please note that a warning is raised and can be turned into an error with a filterwarnings:

```
>>> import warnings
>>> warnings.filterwarnings("error", message=".*check_inverse*.",
... category=UserWarning, append=False)
```

For a full code example that demonstrates using a **FunctionTransformer** to do custom feature selection, see Using FunctionTransformer to select columns