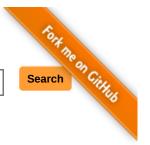


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4.3. Preprocessing data

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.

4.3.1. 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 larç Next

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第1页 共14页 2017/10/24 下午12:32 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:

```
>>>
>>> from sklearn import preprocessing
>>> import numpy as np
>>> X_train = np.array([[ 1., -1., 2.],
               [ 2., 0., 0.],
               [ 0., 1., -1.]])
>>> X_scaled = preprocessing.scale(X_train)
>>> X scaled
array([[ 0. ..., -1.22..., 1.33...],
    [ 1.22..., 0. ..., -0.26...],
    [-1.22..., 1.22..., -1.06...]])
```

Scaled data has zero mean and unit variance:

```
>>>
>>> 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

```
>>>
>>> scaler = preprocessing.StandardScaler().fit(X_train)
StandardScaler(copy=True, with_mean=True, with_std=True)
>>> scaler.mean
array([ 1. ..., 0. ..., 0.33...])
>>> scaler.scale
array([ 0.81..., 0.81..., 1.24...])
>>> scaler.transform(X_train)
array([[ 0. ..., -1.22..., 1.33...],
    [ 1.22..., 0. ..., -0.26...],
    [-1.22..., 1.22..., -1.06...]])
```

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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.

4.3.1.1. 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:

```
>>>
>>> X_train = np.array([[ 1., -1., 2.],
             [ 2., 0., 0.],
             [0., 1., -1.]
>>> min_max_scaler = preprocessing.MinMaxScaler()
>>> X_train_minmax = min_max_scaler.fit_transform(X_train)
>>> X_train_minmax
array([[ 0.5 , 0.
                     , 1.
    [ 1.
           , 0.5 , 0.333333333],
    [ 0.
           , 1.
                   , 0.
```

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:

```
>>>
>>> X test = np.array([[ -3., -1., 4.]])
>>> X_test_minmax = min_max_scaler.transform(X_test)
>>> X_test_minmax
array([[-1.5
            , 0.
                      , 1.66666667]])
```

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第3页 共14页 2017/10/24 下午12:32 It is possible to introspect the scaler attributes to find about the exact nature of the transformation learned on the training data:

```
>>>
>>> min_max_scaler.scale_
array([ 0.5
            , 0.5
                       , 0.33...])
>>> min max scaler.min
                      , 0.33...]
array([ 0.
             , 0.5
```

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:

```
>>>
>>> X_train = np.array([[ 1., -1., 2.],
              [ 2., 0., 0.],
              [ 0., 1., -1.]])
>>> max abs scaler = preprocessing.MaxAbsScaler()
>>> X_train_maxabs = max_abs_scaler.fit_transform(X_train)
>>> X_train_maxabs
                             # doctest +NORMALIZE WHITESPACE
array([[ 0.5, -1. , 1. ],
    [1., 0., 0.],
    [0., 1., -0.5]
>>> X_test = np.array([[ -3., -1., 4.]])
>>> X_test_maxabs = max_abs_scaler.transform(X_test)
>>> X test maxabs
array([[-1.5, -1., 2.]])
>>> max_abs_scaler.scale_
array([ 2., 1., 2.])
```

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

4.3.1.2. Scaling sparse data

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第4页 共14页 2017/10/24 下午12:32 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.

4.3.1.3. 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.

References:

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

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第5页 共14页 2017/10/24 下午12:32 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 or sklearn.decomposition.RandomizedPCA with whiten=True to further remove the linear correlation across features.

Scaling target variables in regression

scale and StandardScaler work out-of-the-box with 1d arrays. This is very useful for scaling the target / response variables used for regression.

4.3.1.4. 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.

4.3.2. Non-linear transformation

Like scalers, QuantileTransformer puts each feature into the same range or distribution. However, by performing a rank transformation, it smooths out unusual distributions and is less influenced by outliers than scaling methods. It does, however, distort correlations and distances within and across features.

QuantileTransformer and quantile transform provide a nonparametric transformation based on the quantile function 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_sta
>>> quantile_transformer = preprocessing.QuantileTransformer(ra
>>> X_train_trans = quantile_transformer.fit_transform(X_train)
>>> X_test_trans = quantile_transformer.transform(X_test)
```

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```
>>> 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...])
```

It is also possible to map the transformed data to a normal distribution by setting output distribution='normal':

```
>>> quantile transformer = preprocessing.QuantileTransformer(>
    output_distribution='normal', random_state=0)
>>> X_trans = quantile_transformer.fit_transform(X)
>>> quantile_transformer.quantiles_
array([[ 4.3..., 2..., 1..., 0.1...],
    [4.31..., 2.02..., 1.01..., 0.1...],
    [4.32..., 2.05..., 1.02..., 0.1...],
    [7.84..., 4.34..., 6.84..., 2.5...],
    [7.87..., 4.37..., 6.87..., 2.5...],
    [7.9..., 4.4..., 6.9..., 2.5...]])
```

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.

4.3.3. 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:

```
>>>
>>> X = [[ 1., -1., 2.],
... [2., 0., 0.],
    [ 0., 1., -1.]]
>>> X_normalized = preprocessing.normalize(X, norm='l2')
>>> X normalized
array([[ 0.40..., -0.40..., 0.81...],
    [1. ..., 0. ..., 0. ...],
    [0. ..., 0.70..., -0.70...]])
```

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
>>> normalizer
Normalizer(copy=True, norm='l2')
```

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

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.

4.3.4. Binarization

4.3.4.1. 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.

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:

```
>>>
>>> X = [[ 1., -1., 2.],
... [2., 0., 0.],
   [ 0., 1., -1.]]
>>> binarizer = preprocessing.Binarizer().fit(X) # fit does nothing
>>> binarizer
Binarizer(copy=True, threshold=0.0)
>>> binarizer.transform(X)
array([[ 1., 0., 1.],
    [1., 0., 0.],
    [0., 1., 0.]])
```

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.

Sparse input

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.

4.3.5. 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].

Such integer representation can not be used directly with 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).

One possibility to convert categorical features to features that can be used with scikit-learn estimators is to use a one-of-K or one-hot encoding, which is implemented in OneHotEncoder. This estimator transforms each categorical feature with m possible values into m binary features, with only one active.

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Continuing the example above:

```
>>>
>>> enc = preprocessing.OneHotEncoder()
>>> enc.fit([[0, 0, 3], [1, 1, 0], [0, 2, 1], [1, 0, 2]])
OneHotEncoder(categorical_features='all', dtype=<... 'numpy.float6
    handle unknown='error', n values='auto', sparse=True)
>>> enc.transform([[0, 1, 3]]).toarray()
array([[ 1., 0., 0., 1., 0., 0., 0., 0., 1.]])
```

By default, how many values each feature can take is inferred automatically from the dataset. It is possible to specify this explicitly using the parameter n_values. There are two genders, three possible continents and four web browsers in our dataset. Then we fit the estimator, and transform a data point. In the result, the first two numbers encode the gender, the next set of three numbers the continent and the last four the web browser.

Note that, if there is a possibility that the training data might have missing categorical features, one has to explicitly set n_values. For example,

```
>>> enc = preprocessing.OneHotEncoder(n values=[2, 3, 4])
>>> # Note that there are missing categorical values for the 2nd ar
>>> # features
>>> enc.fit([[1, 2, 3], [0, 2, 0]])
OneHotEncoder(categorical_features='all', dtype=<... 'numpy.float6
    handle_unknown='error', n_values=[2, 3, 4], sparse=True)
>>> enc.transform([[1, 0, 0]]).toarray()
array([[ 0., 1., 1., 0., 0., 1., 0., 0., 0.]])
```

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

4.3.6. Imputation of missing values

For various reasons, many real world datasets contain missing values, often encoded as blanks, NaNs or other placeholders. Such datasets however are incompatible with scikit-learn estimators which assume that all values in an array are numerical, and that all have and hold meaning. A basic strategy to use incomplete datasets is to discard entire rows and/or columns containing missing values. However, this comes at the price of losing data which may be valuable (even though incomplete). A better strategy is to impute the missing values, i.e., to infer them from the known part of the data.

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第11页 共14页 2017/10/24 下午12:32 The Imputer class provides basic strategies for imputing missing values, either using the mean, the median or the most frequent value of the row or column in which the missing values are located. This class also allows for different missing values encodings.

The following snippet demonstrates how to replace missing values, encoded as np.nan, using the mean value of the columns (axis 0) that contain the missing values:

```
>>>
>>> import numpy as np
>>> from sklearn.preprocessing import Imputer
>>> imp = Imputer(missing_values='NaN', strategy='mean', axis=0)
>>> imp.fit([[1, 2], [np.nan, 3], [7, 6]])
Imputer(axis=0, copy=True, missing_values='NaN', strategy='mean'
>>> X = [[np.nan, 2], [6, np.nan], [7, 6]]
>>> print(imp.transform(X))
[[ 4.
         2.
[ 6.
         3.666...1
[ 7.
         6.
```

The Imputer class also supports sparse matrices:

```
>>>
>>> import scipy.sparse as sp
>>> X = sp.csc_matrix([[1, 2], [0, 3], [7, 6]])
>>> imp = Imputer(missing values=0, strategy='mean', axis=0)
>>> imp.fit(X)
Imputer(axis=0, copy=True, missing_values=0, strategy='mean', ver
>>> X_test = sp.csc_matrix([[0, 2], [6, 0], [7, 6]])
>>> print(imp.transform(X_test))
[[ 4.
         2.
ſ6.
         3.666...1
[ 7.
          6.
```

Note that, here, missing values are encoded by 0 and are thus implicitly stored in the matrix. This format is thus suitable when there are many more missing values than observed values.

Imputer can be used in a Pipeline as a way to build a composite estimator that supports imputation. See Imputing missing values before building an estimator.

4.3.7. 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:

```
>>>
>>> import numpy as np
>>> from sklearn.preprocessing import PolynomialFeatures
>>> X = np.arange(6).reshape(3, 2)
>>> X
array([[0, 1],
    [2, 3],
    [4, 5]])
>>> poly = PolynomialFeatures(2)
>>> poly.fit_transform(X)
array([[ 1., 0., 1., 0., 0., 1.],
    [ 1., 2., 3., 4., 6., 9.],
    [ 1., 4., 5., 16., 20., 25.]])
```

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 = np.arange(9).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., 2., 0., 0., 2., 0.],
    [ 1., 3., 4., 5., 12., 15., 20., 60.],
    [ 1., 6., 7., 8., 42., 48., 56., 336.]])
```

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.

See Polynomial interpolation for Ridge regression using created polynomial features.

4.3.8. Custom transformers

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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 pipeline, do:

```
>>>
>>> import numpy as np
>>> from sklearn.preprocessing import FunctionTransformer
>>> transformer = FunctionTransformer(np.log1p)
>>> X = np.array([[0, 1], [2, 3]])
>>> transformer.transform(X)
array([[ 0. , 0.69314718],
    [ 1.09861229, 1.38629436]])
```

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

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