Python Tutorial 2

January 21, 2020

This tutorial is for Prof. Xin Tong's DSO 530 class at the University of Southern California in spring 2020. It aims to help you to learn how to preprocess the data and build good training sets.

The quality of the data and the amount of useful information that it contains are key factors that determine how well a machine learning algorithm can learn. Therefore, it is absolutely critical that we make sure to examine and preprocess a dataset before we feed it to a learning algorithm. In this tutorial, we will discuss the essential data preprocessing techniques that will help us build good machine learning models.

The topics that we will cover in this tutorial are as follows:
- Removing and imputing missing values from the dataset
- Getting categorical data into shape for machine learning algorithms
- Partitioning a dataset into separate training and test sets
- Bringing features onto the same scale

1 Dealing with missing data

It is not uncommon in real-world applications for our samples to be missing one or more values for various reasons. There could have been an error in the data collection process, certain measurements are not applicable, or particular fields could have been simply left blank in a survey. We typically see missing values as the blank spaces in our data table or as placeholder strings such as *NaN*, which stands for not a number, or *NULL* (a commonly used indicator of unknown values in relational databases).

Unfortunately, most computational tools are unable to handle such missing values, or produce unpredictable results if we simply ignore them. Therefore, it is crucial that we take care of those missing values before we proceed with further analyses. In this section, we will work through several practical techniques for dealing with missing values by removing entries from our dataset or imputing missing values from other samples and features.

1.1 Identifying missing values in tabular data

But before we discuss several techniques for dealing with missing values, let's create a simple example data frame from a **Comma-separated Values (CSV)** file to get a better grasp of the problem:

[1]:
```
import pandas as pd
from io import StringIO
csv_data = \
'''A,B,C,D
```

```
 1.0,2.0,3.0,4.0
 5.0,6.0,,8.0
 10.0,11.0,12.0,'''
df = pd.read_csv(StringIO(csv_data))
df
```

[1]:
```
      A     B     C   D
0   1.0   2.0   3.0  4.0
1   5.0   6.0   NaN  8.0
2  10.0  11.0  12.0  NaN
```

Here, we use *StringIO* to read strings as a file. We also use the backslash (\) to indicate that a statement is continued on the next line. In this way, we split a statement into multiple lines in Python. *A*, *B*, *C* and *D* are different features of the observations.

Using the preceding code, we read CSV-formatted data into a pandas *DataFrame* via the *read_csv* function and noticed that the two missing cells were replaced by NaN. The *StringIO* function in the preceding code example was simply used for the purposes of illustration. It allows us to read the string assigned to *csv_data* into a pandas *DataFrame* as if it was a regular CSV file on our hard drive.

For a larger *DataFrame*, it can be tedious to look for missing values manually; in this case, we can use the *isnull* method to return a *DataFrame* with Boolean values that indicate whether a cell contains a numeric value (*False*) or if data is missing (*True*).

[2]:
```
df.isnull()
```

[2]:
```
       A      B      C      D
0  False  False  False  False
1  False  False   True  False
2  False  False  False   True
```

notnull is the negation of *isnull*.

[3]:
```
df.notnull()
```

[3]:
```
      A     B      C     D
0  True  True   True  True
1  True  True  False  True
2  True  True   True False
```

Using the *sum* method, we can then return the number of missing values per column as follows:

[4]:
```
df.isnull().sum()
```

[4]:
```
A    0
B    0
C    1
D    1
```

```
dtype: int64
```

This way, we can count the number of missing values per column; in the following subsections, we will take a look at different strategies for dealing with these missing data.

P.S. Although scikit-learn was developed for working with NumPy arrays, it can sometimes be more convenient to preprocess data using pandas' *DataFrame*. We can always access the underlying NumPy array of a *DataFrame* via the *values* attribute before we feed it into a scikit-learn estimator:

[5]:
```
df.values
```

[5]:
```
array([[ 1.,  2.,  3.,  4.],
       [ 5.,  6., nan,  8.],
       [10., 11., 12., nan]])
```

The main API implemented by scikit-learn is that of the estimator. An **estimator** is any object that learns from data; it may be a classification, regression or clustering algorithm or a transformer that extracts or filters useful features from raw data.

Note that **estimator** in the field of Statistics means something different.

1.2 Eliminating observations or features with missing values

One of the easiest ways to deal with missing data is to simply remove the corresponding features (columns) or observations (rows) from the dataset entirely; rows with missing values can be easily dropped via the *dropna* method:

[6]:
```
df.dropna(axis=0)
```

[6]:

	A	B	C	D
0	1.0	2.0	3.0	4.0

If we just use *df.dropna()*, it is the same as to specify that *axis = 0*.

Similarly, we can drop columns that have at least one *NaN* in any row by setting the *axis* argument to *1*:

[7]:
```
df.dropna(axis=1)
```

[7]:

	A	B
0	1.0	2.0
1	5.0	6.0
2	10.0	11.0

The *dropna* method supports several additional parameters that can come in handy:

[8]:
```
# only drop rows where all columns are NaN
# (returns the whole array here since we don't
# have a row with where all values are NaN
df.dropna(how='all')
```

[8]:
```
     A     B     C   D
0   1.0   2.0   3.0  4.0
1   5.0   6.0   NaN  8.0
2  10.0  11.0  12.0  NaN
```

[9]:
```
# drop rows that have less than 4 real values
df.dropna(thresh=4)
```

[9]:
```
     A    B    C   D
0  1.0  2.0  3.0  4.0
```

[10]:
```
# only drop rows where NaN appear in specific columns (here: 'C')
df.dropna(subset=['C'])
```

[10]:
```
     A     B     C   D
0   1.0   2.0   3.0  4.0
2  10.0  11.0  12.0  NaN
```

Although the removal of missing data seems to be a convenient approach, it also comes with certain disadvantages; for example, we may end up removing too many observations, which might make reliable analysis impossible. Or, if we remove too many feature columns, we will run the risk of losing valuable information that our classifier needs to discriminate between classes. In the next section, we will thus look at one of the most commonly used alternatives for dealing with missing values: imputation techniques.

1.3 Imputing missing values

1.3.1 Use sklearn.impute.SimpleImputer

https://scikit-learn.org/stable/modules/generated/sklearn.impute.SimpleImputer.html#sklearn.impute.SimpleIm

Often, the removal of entire rows or dropping of entire columns is simply not feasible, because we might lose too much valuable data. In this case, we can use different imputation techniques to estimate the missing values from the other non-null entries in our training data. One of the most common imputation techniques is **mean imputation**, where we simply replace the missing value with the mean value of the entire feature column. A convenient way to achieve this is by using the *SimpleImputer* class from scikit-learn, as shown in the following code:

[11]:
```
import numpy as np
from sklearn.impute import SimpleImputer
imp = SimpleImputer(missing_values = np.nan, strategy = 'mean')
imp = imp.fit(df.values)
imputed_data = imp.transform(df.values)
imputed_data
```

[11]:
```
array([[ 1. ,  2. ,  3. ,  4. ],
       [ 5. ,  6. ,  7.5,  8. ],
       [10. , 11. , 12. ,  6. ]])
```

Here, we replaced each *NaN* value with the corresponding column mean. Other options for the *strategy* parameter are *median*, *constant* or *most_frequent*, where the last replaces the missing values with the most frequent values. This is useful for imputing categorical feature values, for example, a feature column that stores an encoding of color names, such as red, green, and blue, and we will encounter examples of such data later in this tutorial.

When *strategy* == "*constant*", there is another parameter named *fill_value*, which is used to replace all occurrences of missing_values. If left to the default, fill_value will be 0 when imputing numerical data and "missing_value" for strings or object data types.

1.3.2 Use sklearn.impute.KNNImputer

https://scikit-learn.org/stable/modules/generated/sklearn.impute.KNNImputer.html#sklearn-impute-knnimputer

The *KNNImputer* class provides imputation for filling in missing values using the **k-Nearest Neighbors approach**. You can also preview the basic conception of KNN via Wikipedia: https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

Tips

If you cannot import *KNNImputer* from *sklearn.impute* properly, your *sklearn*'s version may not be the latest release. The latest version is 0.22 and you can install the latest version sklearn according to the following website:

https://scikit-learn.org/stable/install.html#install-official-release

or you can try to open the 'Anaconda Prompt' and execute '*conda update –all*' if you are using Anaconda.

By default, a euclidean distance metric that supports missing values, *nan_euclidean_distances*, is used to find the nearest neighbors. Each observation's missing values are imputed using the mean values from *n_neighbors* nearest neighbors found in the training sets. Two observations are close if the features that neither is missing are close.

The following snippet demonstrates how to replace missing values, encoded as *np.nan*, using the mean feature value of the two nearest neighbors of samples with missing values:

[12]:
```
import numpy as np
from sklearn.impute import KNNImputer
X = [[1, 2, np.nan], [3, 4, 3], [np.nan, np.nan, 5], [8, 8, 7]]
df = pd.DataFrame(X, columns=['A', 'B', 'C'])
df
```

[12]:

	A	B	C
0	1.0	2.0	NaN
1	3.0	4.0	3.0
2	NaN	NaN	5.0
3	8.0	8.0	7.0

We set *n_neighbors* to 2, which means that the number of neighboring observations to use for imputation is 2. *n_neighbors*' default value is 5.

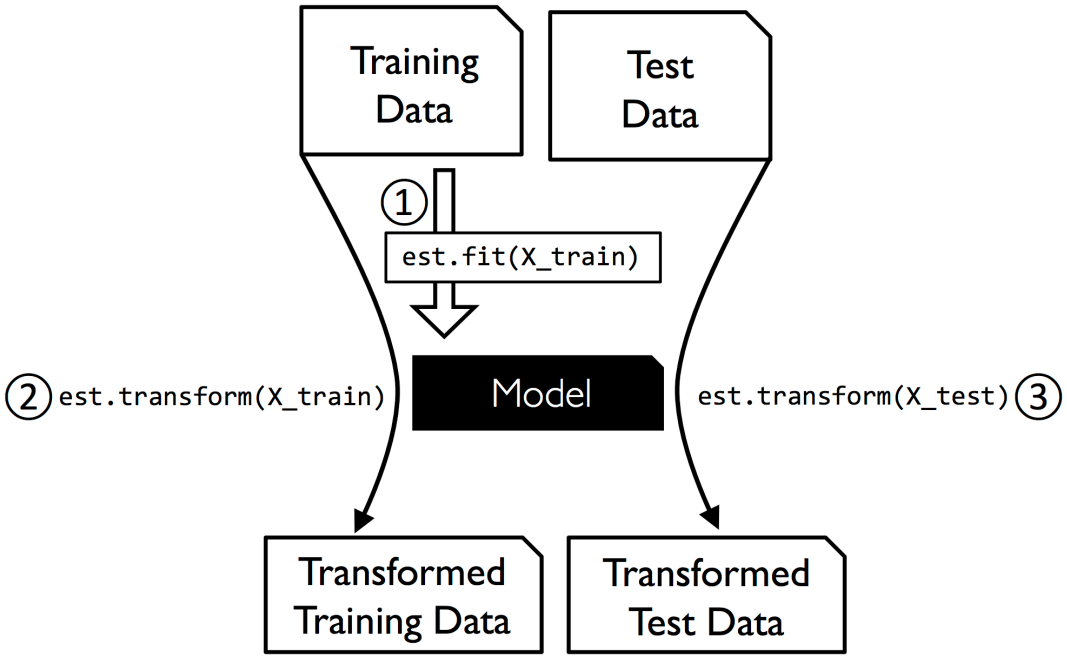
We also set *weights* to "uniform", which means that all points in each neighborhood are weighted equally. Besides, *weights* can be also set to "distance", which means that we weight points by the inverse of their distance. In other word, closer neighbors of a query point will have a greater influence than neighbors which are further away. *weights*' default value is "uniform" :

[13]:
```
imputer = KNNImputer(n_neighbors=2, weights="uniform")
imputer.fit_transform(X)
```

[13]:
```
array([[1. , 2. , 4. ],
       [3. , 4. , 3. ],
       [5.5, 6. , 5. ],
       [8. , 8. , 7. ]])
```

1.4 Understanding the scikit-learn estimator API

In the previous section, we used the *SimpleImputer* and *KNNImputer* class from scikit-learn to impute missing values in our dataset. The *SimpleImputer* and *KNNImputer* class belong to the so-called transformer classes in scikit-learn, which are used for data transformation. The two essential methods of those estimators are *fit* and *transform*. The *fit* method is used to learn the parameters from the training data, and the *transform* method uses those parameters to transform the data. Any data array that is to be transformed needs to have the same number of features as the data array that was used to fit the model. The following figure illustrates how a transformer, fitted on the training data, is used to transform a training dataset as well as a new test dataset:



We give a simple demonstration to show that the missing values of training data and test data are both imputed using the Model trained by training data. The training data is as follows and A, B, C and D are different features of the observations:

[14]:
```
data_train = {'A': [3, 2, np.nan, 4, 3], 'B': [3, np.nan, 4, 4, 5], 'C':[np.
 ↪nan, 4.8, 5.1, 4.9, 5.2], 'D':[6, 7, 9, np.nan, 10]}
df2_train = pd.DataFrame(data = data_train)
df2_train
```

[14]:

	A	B	C	D
0	3.0	3.0	NaN	6.0
1	2.0	NaN	4.8	7.0
2	NaN	4.0	5.1	9.0
3	4.0	4.0	4.9	NaN
4	3.0	5.0	5.2	10.0

The mean of *df2_train* is as follows:

[15]:
```
df2_train.mean(axis = 0)
```

[15]:
```
A    3.0
B    4.0
C    5.0
D    8.0
dtype: float64
```

We use the **mean imputation** technique to impute the missing data. First, we use *fit* to build the model *imp2* (in this case, calculating the mean value of each column in the training data sets), then we use *transform* to impute the missing data in the training data sets. We could see that the imputed values are the mean of each column in the original training data sets.

[16]:
```
imp2 = SimpleImputer(missing_values = np.nan, strategy = 'mean')
imp2 = imp2.fit(df2_train.values)
imputed_df2_train = imp2.transform(df2_train.values)
imputed_df2_train
```

[16]:
```
array([[ 3. ,  3. ,  5. ,  6. ],
       [ 2. ,  4. ,  4.8,  7. ],
       [ 3. ,  4. ,  5.1,  9. ],
       [ 4. ,  4. ,  4.9,  8. ],
       [ 3. ,  5. ,  5.2, 10. ]])
```

Our test data *df2_test* is as follows:

[17]:
```
data_test = {'A': [2, np.nan, 3], 'B': [4, 5, np.nan], 'C':[np.nan, 4, 5], 'D':
 ↪[7, 8, np.nan]}
df2_test = pd.DataFrame(data = data_test)
```

```
df2_test
```

[17]:
```
     A    B    C    D
0  2.0  4.0  NaN  7.0
1  NaN  5.0  4.0  8.0
2  3.0  NaN  5.0  NaN
```

The mean of *df2_test* is as follows:

[18]:
```
df2_test.mean(axis = 0)
```

[18]:
```
A    2.5
B    4.5
C    4.5
D    7.5
dtype: float64
```

Use *imp2.transform* to impute the missing data in the test data sets. We can see that the imputed values are the means of the original training data instead of the test data.

[19]:
```
imputed_df2_test = imp2.transform(df2_test.values)
imputed_df2_test
```

[19]:
```
array([[2., 4., 5., 7.],
       [3., 5., 4., 8.],
       [3., 4., 5., 8.]])
```

2 Handling categorical data

So far, we have only been working with numerical values. However, it is not uncommon that real-world datasets contain one or more categorical feature columns. In this section, we will make use of simple yet effective examples to see how we deal with this type of data in numerical computing libraries.

2.1 Nominal and ordinal features

When we are talking about categorical data, we have to further distinguish between **nominal** and **ordinal** features. Ordinal features can be understood as categorical values that can be sorted or ordered. For example, t-shirt size would be an ordinal feature, because we can define an order $XL > L > M$. In contrast, nominal features don't imply any order and, to continue with the previous example, we could think of t-shirt color as a nominal feature since it typically doesn't make sense to say that, for example, red is larger than blue.

2.1.1 Creating an example dataset

Before we explore different techniques to handle such categorical data, let's create a new *DataFrame* to illustrate the problem:

[20]:
```
import pandas as pd

df = pd.DataFrame([['green', 'M', 10.1, 'class1'],
                   ['red', 'L', 13.5, 'class2'],
                   ['blue', 'XL', 15.3, 'class1']])

df.columns = ['color', 'size', 'price', 'classlabel']
df
```

[20]:

	color	size	price	classlabel
0	green	M	10.1	class1
1	red	L	13.5	class2
2	blue	XL	15.3	class1

As we can see in the preceding output, the newly created DataFrame contains a nominal feature (color), an ordinal feature (size), and a numerical feature (price) column. The class labels (assuming that we created a dataset for a supervised learning task) are stored in the last column.

2.2 Mapping ordinal features

To make sure that the learning algorithm interprets the ordinal features correctly, we need to convert the categorical string values into integers. Unfortunately, there is no convenient function that can automatically derive the correct order of the labels of our *size* feature, so we have to define the mapping manually. In the following simple example, let's assume that we know the numerical difference between features, for example, $XL = L + 1 = M + 2$:

[21]:
```
# we define the mapping manually using the dictionary
size_mapping = {'XL': 3,
                'L': 2,
                'M': 1}

df['size'] = df['size'].map(size_mapping)
df
```

[21]:

	color	size	price	classlabel
0	green	1	10.1	class1
1	red	2	13.5	class2
2	blue	3	15.3	class1

If we want to transform the integer values back to the original string representation at a later stage, we can simply define a reverse-mapping dictionary *inv_size_ mapping = {v: k for k, v in size_mapping.items()}* that can then be used via the pandas map method on the transformed feature column, similar to the size_mapping dictionary that we used previously. We can use it as follows:

[22]:
```
inv_size_mapping = {v: k for k, v in size_mapping.items()}
df['size'].map(inv_size_mapping)
```

[22]:
```
0     M
1     L
2    XL
Name: size, dtype: object
```

P.S. Only domain experts can do this numerical conversion from ordinal to numerical. If we do not know this conversion, we will have to let go of the order information and just convert the variable as if it is just the usual categorical variable, or nominal variable.

2.3 Encoding class labels

Many machine learning libraries require that class labels are encoded as integer values. Although most estimators for classification in scikit-learn convert class labels to integers internally, it is considered good practice to provide class labels as integer arrays to avoid technical glitches. To encode the class labels, we can use an approach similar to the mapping of ordinal features discussed previously. We need to remember that class labels are not ordinal, and it doesn't matter which integer number we assign to a particular string label. Thus, we can simply enumerate the class labels, starting at 0.

There is a convenient *LabelEncoder* class directly implemented in scikit-learn to achieve this:

[23]:
```
from sklearn.preprocessing import LabelEncoder

# Label encoding with sklearn's LabelEncoder
class_le = LabelEncoder()
y = class_le.fit_transform(df['classlabel'].values)
y
```

[23]:
```
array([0, 1, 0])
```

[24]:
```
df['classlabel'] = y
df
```

[24]:

	color	size	price	classlabel
0	green	1	10.1	0
1	red	2	13.5	1
2	blue	3	15.3	0

We can use the *inverse_transform* method to transform the integer class labels back into their original string representation:

[25]:
```
# reverse mapping
df['classlabel'] = class_le.inverse_transform(y)
df
```

[25]:

	color	size	price	classlabel
0	green	1	10.1	class1
1	red	2	13.5	class2
2	blue	3	15.3	class1

Note that the *fit_transform* method is just a shortcut for calling *fit* and *transform* separately:

[26]:
```
class_le2 = LabelEncoder()
class_le2 = class_le2.fit(df['classlabel'].values)
y2 = class_le2.transform(df['classlabel'].values)
y2
```

[26]:
```
array([0, 1, 0])
```

Optional Part in Section 2.3:

We can also use *pandas.Series.map* and *Python Dictionary* to achieve the same thing:

[27]:
```
import numpy as np

# create a mapping dict
# to convert class labels from strings to integers
class_mapping = {label: idx for idx, label in enumerate(np.
 ↪unique(df['classlabel']))}
class_mapping
```

[27]:
```
{'class1': 0, 'class2': 1}
```

Here, *numpy.unique* finds the unique elements of an array. It returns the sorted unique elements of an array.

[28]:
```
np.unique(df['classlabel'])
```

[28]:
```
array(['class1', 'class2'], dtype=object)
```

The Python built-in function *enumerate(iterable)* returns a tuple containing a count (from the start which defaults to 0) and the values obtained from iterating over *iterable*.

[29]:
```
list(enumerate(np.unique(df['classlabel'])))
```

[29]:
```
[(0, 'class1'), (1, 'class2')]
```

Next, we can use the mapping dictionary to transform the class labels into integers:

[30]:
```
# to convert class labels from strings to integers
df['classlabel'] = df['classlabel'].map(class_mapping)
df
```

[30]:

	color	size	price	classlabel
0	green	1	10.1	0
1	red	2	13.5	1
2	blue	3	15.3	0

We can reverse the key-value pairs in the mapping dictionary as follows to map the converted class labels back to the original string representation:

[31]:
```
# reverse the class label mapping
inv_class_mapping = {v: k for k, v in class_mapping.items()}
df['classlabel'] = df['classlabel'].map(inv_class_mapping)
df
```

[31]:

	color	size	price	classlabel
0	green	1	10.1	class1
1	red	2	13.5	class2
2	blue	3	15.3	class1

2.4 Performing one-hot encoding on nominal features

In the previous section, we used a simple dictionary-mapping approach to convert the ordinal *size* feature into integers. Since scikit-learn's estimators for classification treat class labels as categorical data that does not imply any order (nominal), we used the convenient *LabelEncoder* to encode the string labels into integers. It may appear that we could use a similar approach to transform the nominal *color* column of our dataset, as follows:

[32]:
```
X = df[['color', 'size', 'price']].values

X
```

[32]:
```
array([['green', 1, 10.1],
       ['red', 2, 13.5],
       ['blue', 3, 15.3]], dtype=object)
```

[33]:
```
X = df[['color', 'size', 'price']].values

color_le = LabelEncoder()
X[:, 0] = color_le.fit_transform(X[:, 0])
X
```

[33]:
```
array([[1, 1, 10.1],
       [2, 2, 13.5],
       [0, 3, 15.3]], dtype=object)
```

After executing the preceding code, the first column of the NumPy array X now holds the new *color* values, which are encoded as follows:

- blue = 0
- green = 1
- red = 2

If we stop at this point and feed the array to our classifier, we will make one of the most common mistakes in dealing with categorical data. Can you spot the problem? Although the color values don't come in any particular order, a learning algorithm will now assume that *green* is larger than *blue*, and *red* is larger than *green*.

A common workaround for this problem is to use a technique called one-hot encoding. The idea behind this approach is to create a new dummy feature for each unique value in the nominal feature column. Here, we would convert the color feature into three new features: *blue*, *green*, and *red*. Binary values can then be used to indicate the particular *color* of a sample; for example, a blue t-shirt can be encoded as *blue=1, green=0, red=0*. To perform this transformation, we can use the *OneHotEncoder* that is implemented in the *scikit-learn.preprocessing* module and we also need to import *ColumnTransformer* from *sklearn.compose* to specify which column to transform. Here we use *ColumnTransformer* to specify that we are transforming the *[0]* column :

[34]:
```
from sklearn.preprocessing import OneHotEncoder
from sklearn.compose import ColumnTransformer

ct = ColumnTransformer([("color", OneHotEncoder(), [0])], remainder =␣
↪'passthrough')
X = ct.fit_transform(X)

X
```

[34]:
```
array([[0.0, 1.0, 0.0, 1, 10.1],
       [0.0, 0.0, 1.0, 2, 13.5],
       [1.0, 0.0, 0.0, 3, 15.3]], dtype=object)
```

An even more convenient way to create those dummy features via one-hot encoding is to use the *get_dummies* method implemented in pandas. Applied to a *DataFrame*, the *get_dummies* method will only convert string columns and leave all other columns unchanged:

[35]:
```
# one-hot encoding via pandas
pd.get_dummies(df[['price', 'color', 'size']])
```

[35]:

	price	size	color_blue	color_green	color_red
0	10.1	1	0	1	0
1	13.5	2	0	0	1
2	15.3	3	1	0	0

When we are using one-hot encoding datasets, we have to keep in mind that it introduces multicollinearity, which can be an issue for certain methods (for instance, methods that require matrix inversion). If features are highly correlated, matrices are computationally difficult to invert, which can lead to numerically unstable estimates. To reduce the correlation among variables, we can simply remove one feature column from the one-hot encoded array. Note that we do not lose any important information by removing a feature column, though; for example, if we remove the column *color_blue*, the feature information is still preserved since if we observe *color_green=0* and *color_red=0*, it implies that the observation must be *blue*. For a nominal variable with *K* categories, we only need *K-1* dummies.

If we use the *get_dummies* function, we can drop the first column by passing a *True* argument to the *drop_first* parameter, as shown in the following code example:

[36]:
```
# multicollinearity guard in get_dummies
pd.get_dummies(df[['price', 'color', 'size']], drop_first=True)
```

[36]:

	price	size	color_green	color_red
0	10.1	1	1	0
1	13.5	2	0	1
2	15.3	3	0	0

If we use the *OneHotEncoder* and *ColumnTransformer* function, we can drop the first column by passing a *first* argument to the *drop* parameter in *OneHotEncoder*, as shown in the following code example:

[37]:
```
ct = ColumnTransformer([("color", OneHotEncoder(drop = 'first'), [0])],␣
↪remainder = 'passthrough')
X = ct.fit_transform(X)

X
```

[37]:
```
array([[1.0, 0.0, 1, 10.1],
       [0.0, 1.0, 2, 13.5],
       [0.0, 0.0, 3, 15.3]], dtype=object)
```

3 Partitioning a dataset into separate training and test sets

We aim to build a machine learning model from some data that can achieve our goal. But before we can apply our model to new measurements, we need to know whether it actually works—that is, whether we should trust its predictions.

Unfortunately, we cannot use the data we used to build the model to evaluate it. This is because our model can always simply remember the whole training set, and will therefore always predict the correct label for any point in the training set. This "remembering" does not indicate to us whether our model will generalize well (in other words, whether it will also perform well on new data).

To assess the model's performance, we show it new data (data that it hasn't seen before) for which we have labels. This is usually done by splitting the labeled data we have collected into two parts. One part of the data is used to build our machine learning model, and is called the **training data** or **training set**. The rest of the data will be used to assess how well the model works; this is called the **test data**, **test set**, or **hold-out set**.

In this section, we will prepare a new dataset, the **Wine** dataset. After we have preprocessed the dataset, we will explore different techniques for feature selection to reduce the dimensionality of a dataset.

The Wine dataset is another open-source dataset that is available from the UCI machine learning repository (https://archive.ics.uci.edu/ml/datasets/Wine); it consists of 178 wine observations with 13 features describing their different chemical properties.

Using the pandas library, we will directly read in the open-source Wine dataset from the UCI machine learning repository:

[38]:
```
df_wine = pd.read_csv('https://archive.ics.uci.edu/ml/'␣
 ↪'machine-learning-databases/wine/wine.data', header=None)

# if the Wine dataset is temporarily unavailable from the
# UCI machine learning repository, un-comment the following line
# of code to load the dataset from a local path:

# df_wine = pd.read_csv('wine.data', header=None)

df_wine.columns = ['Class label', 'Alcohol', 'Malic acid', 'Ash',
                   'Alcalinity of ash', 'Magnesium', 'Total phenols',
                   'Flavanoids', 'Nonflavanoid phenols', 'Proanthocyanins',
                   'Color intensity', 'Hue', 'OD280/OD315 of diluted wines',
                   'Proline']

print('Class labels', np.unique(df_wine['Class label']))
df_wine.head()
```

```
Class labels [1 2 3]
```

[38]:

	Class label	Alcohol	Malic acid	Ash	Alcalinity of ash	Magnesium	\
0	1	14.23	1.71	2.43	15.6	127	
1	1	13.20	1.78	2.14	11.2	100	
2	1	13.16	2.36	2.67	18.6	101	
3	1	14.37	1.95	2.50	16.8	113	
4	1	13.24	2.59	2.87	21.0	118	

	Total phenols	Flavanoids	Nonflavanoid phenols	Proanthocyanins	\
0	2.80	3.06	0.28	2.29	
1	2.65	2.76	0.26	1.28	
2	2.80	3.24	0.30	2.81	
3	3.85	3.49	0.24	2.18	
4	2.80	2.69	0.39	1.82	

	Color intensity	Hue	OD280/OD315 of diluted wines	Proline
0	5.64	1.04	3.92	1065
1	4.38	1.05	3.40	1050
2	5.68	1.03	3.17	1185
3	7.80	0.86	3.45	1480
4	4.32	1.04	2.93	735

The 13 different features in the Wine dataset, describing the chemical properties of the 178 wine samples, are listed in the above table.

A bottle of wine in the collection belongs to one of three different classes, 1, 2, and 3, which refer to the three different types of grape grown in the same region in Italy but derived from different wine cultivars, as described in the dataset summary (https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.names).

A convenient way to randomly partition this dataset into separate test and training datasets is to use the *train_test_split* function from scikit-learn's *model_selection* submodule:

[39]:
```
from sklearn.model_selection import train_test_split

X, y = df_wine.iloc[:, 1:].values, df_wine.iloc[:, 0].values

X_train, X_test, y_train, y_test =\
    train_test_split(X, y,
                     test_size=0.3,
                     random_state=0,
                     stratify=y)
```

First, we assigned the NumPy array representation of the feature columns 1-13 to the variable X; we assigned the class labels from the first column to the variable y. Then, we used the *train_test_split* function to randomly split X and y into separate training and test datasets. By setting *test_size=0.3* (the default value of *test_size* is 0.25), we assigned 30 percent of the wine samples to *X_test* and *y_test*, and the remaining 70 percent of the samples were assigned to *X_train* and *y_train*, respectively. We use the *random_state* parameter to set the random seed, which is important for the reproducibility of the results. Providing the class label array y as an argument to *stratify* ensures that both training and test datasets have the same class proportions as the original dataset.

P.S. If we are dividing a dataset into training and test datasets, we have to keep in mind that we are withholding valuable information that the learning algorithm could benefit from. Thus, we don't want to allocate too much information on the test set. However, the smaller the test set, the more inaccurate the estimation of the generalization error. Dividing a dataset into training and test sets is all about balancing this trade-off. In practice, the most commonly used splits are 60:40, 70:30, or 80:20, depending on the size of the initial dataset. However, for large datasets, 90:10 or 99:1 splits into training and test subsets are also common and appropriate. Instead of discarding the allocated test data after model training and evaluation, it is a common practice to retrain a classifier on the entire dataset as it can improve the predictive performance of the model.

4 Bringing features onto the same scale

Feature scaling is a crucial step in our preprocessing pipeline that can easily be forgotten. In this tutorial, we will not discuss when and where we should take a feature scaling step because whether bringing different features onto the same scale can improve our model is subtle and that even should be discussed case in case. Here we only introduce two approaches to feature scaling.

Now, there are two common approaches to bring different features onto the same scale: **normalization** and **standardization**. Those terms are often used quite loosely in different fields, and the meaning has to be derived from the context. Most often, **normalization** refers to the rescaling of the features to a range of [0, 1], which is a special case of **min-max scaling**. To normalize our data, we can simply apply the min-max scaling to each feature column, where the new value $x^{(i)}_{norm}$ of a sample $x^{(i)}$ can be calculated as follows:

$$x^{(i)}_{norm} = \frac{x^{(i)} - x_{min}}{x_{max} - x_{min}}$$

Here, $x^{(i)}$ is the i-th observation, x_{min} is the smallest value in a feature column, and x_{max} is the

largest value.

The **min-max scaling** procedure is implemented in scikit-learn and can be used as follows:

[40]:
```
from sklearn.preprocessing import MinMaxScaler

mms = MinMaxScaler()
X_train_norm = mms.fit_transform(X_train)
X_test_norm = mms.transform(X_test)
```

P.S. Note that if x_{min} in the test data is smaller than x_{min} in the training data, then the transformed test point might have a value smaller than 0.

[41]:
```
ex_train = np.array([3, 4, 5, 6, 7, 8]).reshape(6, 1)
ex_train
```

[41]:
```
array([[3],
       [4],
       [5],
       [6],
       [7],
       [8]])
```

[42]:
```
mms_ex = MinMaxScaler()
ex_train_norm = mms_ex.fit_transform(ex_train)
ex_train_norm
```

[42]:
```
array([[0. ],
       [0.2],
       [0.4],
       [0.6],
       [0.8],
       [1. ]])
```

[43]:
```
ex_test = np.array([2, 3, 4, 5]).reshape(4, 1)
ex_test
```

[43]:
```
array([[2],
       [3],
       [4],
       [5]])
```

[44]:
```
ex_test_norm = mms_ex.transform(ex_test)
ex_test_norm
```

[44]:
```
array([[-0.2],
       [ 0. ],
       [ 0.2],
```

```
 [ 0.4]])
```

Using **standardization**, we center the feature columns at mean 0 with standard deviation 1 so that the feature columns take the form of a normal distribution, which makes it easier to learn the weights. Furthermore, standardization maintains useful information about outliers and makes the algorithm less sensitive to them in contrast to min-max scaling, which scales the data to a limited range of values.

The procedure for **standardization** can be expressed by the following equation:

$$x_{std}^{(i)} = \frac{x^{(i)} - \mu_x}{\sigma_x}$$

Here, μ_x is the sample mean of a particular feature column and σ_x corresponding standard deviation.

Similar to the *MinMaxScaler* class, scikit-learn also implements a class for **standardization**:

[45]:
```
from sklearn.preprocessing import StandardScaler

stdsc = StandardScaler()
X_train_std = stdsc.fit_transform(X_train)
X_test_std = stdsc.transform(X_test)
```

Again, it is also important to highlight that we fit the StandardScaler class only once—on the training data—and use those parameters to transform the test set or any new data point.

The following table illustrates the difference between the two commonly used feature scaling techniques, standardization and normalization, on a simple sample dataset consisting of numbers 0 to 5:

Input	Standardized	Min-max normalized
0.0	-1.46385	0.0
1.0	-0.87831	0.2
2.0	-0.29277	0.4
3.0	0.29277	0.6
4.0	0.87831	0.8
5.0	1.46385	1.0

You can perform the standardization and normalization shown in the table manually by executing the following code examples:

[46]:
```
ex = np.array([0, 1, 2, 3, 4, 5])
ex
```

[46]:
```
array([0, 1, 2, 3, 4, 5])
```

stdsc.fit_transform and *mms.fit_transform* both expect 2D array, but ex is an 1D array. Thus, we use *array.reshape (-1,1)* to reshape the 1D array to a 2D array.

array.reshape (-1,k) means that we reshape the array into k columns and the number of rows will be inferred automatically. Similarly, *array.reshape (k,-1)* means that we reshape the array into k

rows and the number of columns will be inferred automatically.

[47]:
```
ex_std = stdsc.fit_transform(ex.reshape(-1,1))
ex_norm = mms.fit_transform(ex.reshape(-1, 1))
print('standardized:', ex_std.reshape(1,-1))
print('normalized:', ex_norm.reshape(1,-1))
```

```
standardized: [[-1.46385011 -0.87831007 -0.29277002  0.29277002  0.87831007
1.46385011]]
normalized: [[0.  0.2 0.4 0.6 0.8 1. ]]
```

We can use the formula of definition to validate the results:

[48]:
```
print('standardized:', (ex - ex.mean()) / ex.std())
print('normalized:', (ex - ex.min()) / (ex.max() - ex.min()))
```

```
standardized: [-1.46385011 -0.87831007 -0.29277002  0.29277002  0.87831007
1.46385011]
normalized: [0.  0.2 0.4 0.6 0.8 1. ]
```

References:

Müller, Andreas C; Guido, Sarah. (2017). Introduction to Machine Learning with Python.

Raschka, S. (2017). Python Machine Learning.

https://scikit-learn.org/stable/index.html

https://archive.ics.uci.edu/ml/datasets.php

https://en.wikipedia.org/wiki/