CHAPTER 13

Introduction to Modeling Libraries in Python

In this book, I have focused on providing a programming foundation for doing data analysis in Python. Since data analysts and scientists often report spending a disproportionate amount of time with data wrangling and preparation, the book's structure reflects the importance of mastering these techniques.

Which library you use for developing models will depend on the application. Many statistical problems can be solved by simpler techniques like ordinary least squares regression, while other problems may call for more advanced machine learning methods. Fortunately, Python has become one of the languages of choice for implementing analytical methods, so there are many tools you can explore after completing this book.

In this chapter, I will review some features of pandas that may be helpful when you're crossing back and forth between data wrangling with pandas and model fitting and scoring. I will then give short introductions to two popular modeling toolkits, statsmodels and scikit-learn. Since each of these projects is large enough to warrant its own dedicated book, I make no effort to be comprehensive and instead direct you to both projects' online documentation along with some other Python-based books on data science, statistics, and machine learning.

13.1 Interfacing Between pandas and Model Code

A common workflow for model development is to use pandas for data loading and cleaning before switching over to a modeling library to build the model itself. An important part of the model development process is called *feature engineering* in machine learning. This can describe any data transformation or analytics that extract information from a raw dataset that may be useful in a modeling context. The data aggregation and GroupBy tools we have explored in this book are used often in a feature engineering context.

While details of "good" feature engineering are out of scope for this book, I will show some methods to make switching between data manipulation with pandas and modeling as painless as possible.

The point of contact between pandas and other analysis libraries is usually NumPy arrays. To turn a DataFrame into a NumPy array, use the `.values` property:

```
In [10]: import pandas as pd

In [11]: import numpy as np

In [12]: data = pd.DataFrame({
   ....:     'x0': [1, 2, 3, 4, 5],
   ....:     'x1': [0.01, -0.01, 0.25, -4.1, 0.],
   ....:     'y': [-1.5, 0., 3.6, 1.3, -2.]})

In [13]: data
Out[13]:
   x0    x1    y
0   1  0.01 -1.5
1   2 -0.01  0.0
2   3  0.25  3.6
3   4 -4.10  1.3
4   5  0.00 -2.0

In [14]: data.columns
Out[14]: Index(['x0', 'x1', 'y'], dtype='object')

In [15]: data.values
Out[15]:
array([[ 1.  ,  0.01, -1.5 ],
       [ 2.  , -0.01,  0.  ],
       [ 3.  ,  0.25,  3.6 ],
       [ 4.  , -4.1 ,  1.3 ],
       [ 5.  ,  0.  , -2.  ]])
```

To convert back to a DataFrame, as you may recall from earlier chapters, you can pass a two-dimensional ndarray with optional column names:

```
In [16]: df2 = pd.DataFrame(data.values, columns=['one', 'two', 'three'])

In [17]: df2
Out[17]:
   one   two  three
0  1.0  0.01   -1.5
1  2.0 -0.01    0.0
2  3.0  0.25    3.6
```

```
3  4.0 -4.10   1.3
4  5.0  0.00  -2.0
```

The `.values` attribute is intended to be used when your data is homogeneous—for example, all numeric types. If you have heterogeneous data, the result will be an ndarray of Python objects:

```
In [18]: df3 = data.copy()

In [19]: df3['strings'] = ['a', 'b', 'c', 'd', 'e']

In [20]: df3
Out[20]:
   x0    x1    y strings
0   1  0.01 -1.5       a
1   2 -0.01  0.0       b
2   3  0.25  3.6       c
3   4 -4.10  1.3       d
4   5  0.00 -2.0       e

In [21]: df3.values
Out[21]:
array([[1, 0.01, -1.5, 'a'],
       [2, -0.01, 0.0, 'b'],
       [3, 0.25, 3.6, 'c'],
       [4, -4.1, 1.3, 'd'],
       [5, 0.0, -2.0, 'e']], dtype=object)
```

For some models, you may only wish to use a subset of the columns. I recommend using `loc` indexing with `values`:

```
In [22]: model_cols = ['x0', 'x1']

In [23]: data.loc[:, model_cols].values
Out[23]:
array([[ 1.  ,  0.01],
       [ 2.  , -0.01],
       [ 3.  ,  0.25],
       [ 4.  , -4.1 ],
       [ 5.  ,  0.  ]])
```

Some libraries have native support for pandas and do some of this work for you automatically: converting to NumPy from DataFrame and attaching model parameter names to the columns of output tables or Series. In other cases, you will have to perform this "metadata management" manually.

In Chapter 12 we looked at pandas's `Categorical` type and the `pandas.get_dummies` function. Suppose we had a non-numeric column in our example dataset:

```
In [24]: data['category'] = pd.Categorical(['a', 'b', 'a', 'a', 'b'],
   ....:                                   categories=['a', 'b'])

In [25]: data
Out[25]: 
   x0    x1    y category
0   1  0.01 -1.5        a
1   2 -0.01  0.0        b
2   3  0.25  3.6        a
3   4 -4.10  1.3        a
4   5  0.00 -2.0        b
```

If we wanted to replace the `'category'` column with dummy variables, we create dummy variables, drop the `'category'` column, and then join the result:

```
In [26]: dummies = pd.get_dummies(data.category, prefix='category')

In [27]: data_with_dummies = data.drop('category', axis=1).join(dummies)

In [28]: data_with_dummies
Out[28]: 
   x0    x1    y  category_a  category_b
0   1  0.01 -1.5           1           0
1   2 -0.01  0.0           0           1
2   3  0.25  3.6           1           0
3   4 -4.10  1.3           1           0
4   5  0.00 -2.0           0           1
```

There are some nuances to fitting certain statistical models with dummy variables. It may be simpler and less error-prone to use Patsy (the subject of the next section) when you have more than simple numeric columns.

13.2 Creating Model Descriptions with Patsy

Patsy is a Python library for describing statistical models (especially linear models) with a small string-based "formula syntax," which is inspired by (but not exactly the same as) the formula syntax used by the R and S statistical programming languages.

Patsy is well supported for specifying linear models in statsmodels, so I will focus on some of the main features to help you get up and running. Patsy's *formulas* are a special string syntax that looks like:

```
y ~ x0 + x1
```

The syntax `a + b` does not mean to add `a` to `b`, but rather that these are *terms* in the *design matrix* created for the model. The `patsy.dmatrices` function takes a formula string along with a dataset (which can be a DataFrame or a dict of arrays) and produces design matrices for a linear model:

```
In [29]: data = pd.DataFrame({
   ....:     'x0': [1, 2, 3, 4, 5],
```

```
   ....:     'x1': [0.01, -0.01, 0.25, -4.1, 0.],
   ....:     'y': [-1.5, 0., 3.6, 1.3, -2.]})

In [30]: data
Out[30]:
   x0    x1    y
0   1  0.01 -1.5
1   2 -0.01  0.0
2   3  0.25  3.6
3   4 -4.10  1.3
4   5  0.00 -2.0

In [31]: import patsy

In [32]: y, X = patsy.dmatrices('y ~ x0 + x1', data)
```

Now we have:

```
In [33]: y
Out[33]:
DesignMatrix with shape (5, 1)
     y
  -1.5
   0.0
   3.6
   1.3
  -2.0
  Terms:
    'y' (column 0)

In [34]: X
Out[34]:
DesignMatrix with shape (5, 3)
  Intercept  x0     x1
          1   1   0.01
          1   2  -0.01
          1   3   0.25
          1   4  -4.10
          1   5   0.00
  Terms:
    'Intercept' (column 0)
    'x0' (column 1)
    'x1' (column 2)
```

These Patsy `DesignMatrix` instances are NumPy ndarrays with additional metadata:

```
In [35]: np.asarray(y)
Out[35]:
array([[-1.5],
       [ 0. ],
       [ 3.6],
       [ 1.3],
       [-2. ]])
```

```
In [36]: np.asarray(X)
Out[36]:
array([[ 1.  ,  1.  ,  0.01],
       [ 1.  ,  2.  , -0.01],
       [ 1.  ,  3.  ,  0.25],
       [ 1.  ,  4.  , -4.1 ],
       [ 1.  ,  5.  ,  0.  ]])
```

You might wonder where the `Intercept` term came from. This is a convention for linear models like ordinary least squares (OLS) regression. You can suppress the intercept by adding the term `+ 0` to the model:

```
In [37]: patsy.dmatrices('y ~ x0 + x1 + 0', data)[1]
Out[37]:
DesignMatrix with shape (5, 2)
  x0     x1
   1   0.01
   2  -0.01
   3   0.25
   4  -4.10
   5   0.00
  Terms:
    'x0' (column 0)
    'x1' (column 1)
```

The Patsy objects can be passed directly into algorithms like `numpy.linalg.lstsq`, which performs an ordinary least squares regression:

```
In [38]: coef, resid, _, _ = np.linalg.lstsq(X, y)
```

The model metadata is retained in the `design_info` attribute, so you can reattach the model column names to the fitted coefficients to obtain a Series, for example:

```
In [39]: coef
Out[39]:
array([[ 0.3129],
       [-0.0791],
       [-0.2655]])

In [40]: coef = pd.Series(coef.squeeze(), index=X.design_info.column_names)

In [41]: coef
Out[41]:
Intercept    0.312910
x0          -0.079106
x1          -0.265464
dtype: float64
```

Data Transformations in Patsy Formulas

You can mix Python code into your Patsy formulas; when evaluating the formula the library will try to find the functions you use in the enclosing scope:

```
In [42]: y, X = patsy.dmatrices('y ~ x0 + np.log(np.abs(x1) + 1)', data)

In [43]: X
Out[43]:
DesignMatrix with shape (5, 3)
  Intercept  x0  np.log(np.abs(x1) + 1)
          1   1                 0.00995
          1   2                 0.00995
          1   3                 0.22314
          1   4                 1.62924
          1   5                 0.00000
  Terms:
    'Intercept' (column 0)
    'x0' (column 1)
    'np.log(np.abs(x1) + 1)' (column 2)
```

Some commonly used variable transformations include standardizing (to mean 0 and variance 1) and centering (subtracting the mean). Patsy has built-in functions for this purpose:

```
In [44]: y, X = patsy.dmatrices('y ~ standardize(x0) + center(x1)', data)

In [45]: X
Out[45]:
DesignMatrix with shape (5, 3)
  Intercept  standardize(x0)  center(x1)
          1         -1.41421        0.78
          1         -0.70711        0.76
          1          0.00000        1.02
          1          0.70711       -3.33
          1          1.41421        0.77
  Terms:
    'Intercept' (column 0)
    'standardize(x0)' (column 1)
    'center(x1)' (column 2)
```

As part of a modeling process, you may fit a model on one dataset, then evaluate the model based on another. This might be a *hold-out* portion or new data that is observed later. When applying transformations like center and standardize, you should be careful when using the model to form predications based on new data. These are called *stateful* transformations, because you must use statistics like the mean or standard deviation of the original dataset when transforming a new dataset.

The `patsy.build_design_matrices` function can apply transformations to new *out-of-sample* data using the saved information from the original *in-sample* dataset:

```
In [46]: new_data = pd.DataFrame({
   ....:     'x0': [6, 7, 8, 9],
   ....:     'x1': [3.1, -0.5, 0, 2.3],
   ....:     'y': [1, 2, 3, 4]})

In [47]: new_X = patsy.build_design_matrices([X.design_info], new_data)

In [48]: new_X
Out[48]:
[DesignMatrix with shape (4, 3)
   Intercept  standardize(x0)  center(x1)
           1          2.12132        3.87
           1          2.82843        0.27
           1          3.53553        0.77
           1          4.24264        3.07
   Terms:
     'Intercept' (column 0)
     'standardize(x0)' (column 1)
     'center(x1)' (column 2)]
```

Because the plus symbol (+) in the context of Patsy formulas does not mean addition, when you want to add columns from a dataset by name, you must wrap them in the special *I* function:

```
In [49]: y, X = patsy.dmatrices('y ~ I(x0 + x1)', data)

In [50]: X
Out[50]:
DesignMatrix with shape (5, 2)
  Intercept  I(x0 + x1)
          1        1.01
          1        1.99
          1        3.25
          1       -0.10
          1        5.00
  Terms:
    'Intercept' (column 0)
    'I(x0 + x1)' (column 1)
```

Patsy has several other built-in transforms in the `patsy.builtins` module. See the online documentation for more.

Categorical data has a special class of transformations, which I explain next.

Categorical Data and Patsy

Non-numeric data can be transformed for a model design matrix in many different ways. A complete treatment of this topic is outside the scope of this book and would be best studied along with a course in statistics.

When you use non-numeric terms in a Patsy formula, they are converted to dummy variables by default. If there is an intercept, one of the levels will be left out to avoid collinearity:

```
In [51]: data = pd.DataFrame({
   ....:     'key1': ['a', 'a', 'b', 'b', 'a', 'b', 'a', 'b'],
   ....:     'key2': [0, 1, 0, 1, 0, 1, 0, 0],
   ....:     'v1': [1, 2, 3, 4, 5, 6, 7, 8],
   ....:     'v2': [-1, 0, 2.5, -0.5, 4.0, -1.2, 0.2, -1.7]
   ....: })

In [52]: y, X = patsy.dmatrices('v2 ~ key1', data)

In [53]: X
Out[53]:
DesignMatrix with shape (8, 2)
  Intercept  key1[T.b]
          1          0
          1          0
          1          1
          1          1
          1          0
          1          1
          1          0
          1          1
  Terms:
    'Intercept' (column 0)
    'key1' (column 1)
```

If you omit the intercept from the model, then columns for each category value will be included in the model design matrix:

```
In [54]: y, X = patsy.dmatrices('v2 ~ key1 + 0', data)

In [55]: X
Out[55]:
DesignMatrix with shape (8, 2)
  key1[a]  key1[b]
        1        0
        1        0
        0        1
        0        1
        1        0
        0        1
        1        0
        0        1
  Terms:
    'key1' (columns 0:2)
```

Numeric columns can be interpreted as categorical with the `C` function:

```
In [56]: y, X = patsy.dmatrices('v2 ~ C(key2)', data)
```

```
In [57]: X
Out[57]:
DesignMatrix with shape (8, 2)
  Intercept  C(key2)[T.1]
          1             0
          1             1
          1             0
          1             1
          1             0
          1             1
          1             0
          1             0
  Terms:
    'Intercept' (column 0)
    'C(key2)' (column 1)
```

When you're using multiple categorical terms in a model, things can be more complicated, as you can include interaction terms of the form `key1:key2`, which can be used, for example, in analysis of variance (ANOVA) models:

```
In [58]: data['key2'] = data['key2'].map({0: 'zero', 1: 'one'})

In [59]: data
Out[59]:
  key1  key2  v1   v2
0    a  zero   1 -1.0
1    a   one   2  0.0
2    b  zero   3  2.5
3    b   one   4 -0.5
4    a  zero   5  4.0
5    b   one   6 -1.2
6    a  zero   7  0.2
7    b  zero   8 -1.7

In [60]: y, X = patsy.dmatrices('v2 ~ key1 + key2', data)

In [61]: X
Out[61]:
DesignMatrix with shape (8, 3)
  Intercept  key1[T.b]  key2[T.zero]
          1          0             1
          1          0             0
          1          1             1
          1          1             0
          1          0             1
          1          1             0
          1          0             1
          1          1             1
  Terms:
    'Intercept' (column 0)
    'key1' (column 1)
    'key2' (column 2)
```

```
In [62]: y, X = patsy.dmatrices('v2 ~ key1 + key2 + key1:key2', data)

In [63]: X
Out[63]:
DesignMatrix with shape (8, 4)
  Intercept  key1[T.b]  key2[T.zero]  key1[T.b]:key2[T.zero]
          1          0             1                       0
          1          0             0                       0
          1          1             1                       1
          1          1             0                       0
          1          0             1                       0
          1          1             0                       0
          1          0             1                       0
          1          1             1                       1
  Terms:
    'Intercept' (column 0)
    'key1' (column 1)
    'key2' (column 2)
    'key1:key2' (column 3)
```

Patsy provides for other ways to transform categorical data, including transformations for terms with a particular ordering. See the online documentation for more.

13.3 Introduction to statsmodels

statsmodels is a Python library for fitting many kinds of statistical models, performing statistical tests, and data exploration and visualization. Statsmodels contains more "classical" frequentist statistical methods, while Bayesian methods and machine learning models are found in other libraries.

Some kinds of models found in statsmodels include:

- Linear models, generalized linear models, and robust linear models
- Linear mixed effects models
- Analysis of variance (ANOVA) methods
- Time series processes and state space models
- Generalized method of moments

In the next few pages, we will use a few basic tools in statsmodels and explore how to use the modeling interfaces with Patsy formulas and pandas DataFrame objects.

Estimating Linear Models

There are several kinds of linear regression models in statsmodels, from the more basic (e.g., ordinary least squares) to more complex (e.g., iteratively reweighted least squares).

Linear models in statsmodels have two different main interfaces: array-based and formula-based. These are accessed through these API module imports:

```
import statsmodels.api as sm
import statsmodels.formula.api as smf
```

To show how to use these, we generate a linear model from some random data:

```
def dnorm(mean, variance, size=1):
    if isinstance(size, int):
        size = size,
    return mean + np.sqrt(variance) * np.random.randn(*size)

# For reproducibility
np.random.seed(12345)

N = 100
X = np.c_[dnorm(0, 0.4, size=N),
          dnorm(0, 0.6, size=N),
          dnorm(0, 0.2, size=N)]
eps = dnorm(0, 0.1, size=N)
beta = [0.1, 0.3, 0.5]

y = np.dot(X, beta) + eps
```

Here, I wrote down the "true" model with known parameters `beta`. In this case, `dnorm` is a helper function for generating normally distributed data with a particular mean and variance. So now we have:

```
In [66]: X[:5]
Out[66]:
array([[-0.1295, -1.2128,  0.5042],
       [ 0.3029, -0.4357, -0.2542],
       [-0.3285, -0.0253,  0.1384],
       [-0.3515, -0.7196, -0.2582],
       [ 1.2433, -0.3738, -0.5226]])

In [67]: y[:5]
Out[67]: array([ 0.4279, -0.6735, -0.0909, -0.4895, -0.1289])
```

A linear model is generally fitted with an intercept term as we saw before with Patsy. The `sm.add_constant` function can add an intercept column to an existing matrix:

```
In [68]: X_model = sm.add_constant(X)

In [69]: X_model[:5]
Out[69]:
array([[ 1.    , -0.1295, -1.2128,  0.5042],
       [ 1.    ,  0.3029, -0.4357, -0.2542],
       [ 1.    , -0.3285, -0.0253,  0.1384],
       [ 1.    , -0.3515, -0.7196, -0.2582],
       [ 1.    ,  1.2433, -0.3738, -0.5226]])
```

The sm.OLS class can fit an ordinary least squares linear regression:

```
In [70]: model = sm.OLS(y, X)
```

The model's fit method returns a regression results object containing estimated model parameters and other diagnostics:

```
In [71]: results = model.fit()

In [72]: results.params
Out[72]: array([ 0.1783,  0.223 ,  0.501 ])
```

The summary method on results can print a model detailing diagnostic output of the model:

```
In [73]: print(results.summary())
OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.430
Model:                            OLS   Adj. R-squared:                  0.413
Method:                 Least Squares   F-statistic:                     24.42
Date:                Mon, 25 Sep 2017   Prob (F-statistic):           7.44e-12
Time:                        14:06:15   Log-Likelihood:                -34.305
No. Observations:                 100   AIC:                             74.61
Df Residuals:                      97   BIC:                             82.42
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
x1             0.1783      0.053      3.364      0.001       0.073       0.283
x2             0.2230      0.046      4.818      0.000       0.131       0.315
x3             0.5010      0.080      6.237      0.000       0.342       0.660
==============================================================================
Omnibus:                        4.662   Durbin-Watson:                   2.201
Prob(Omnibus):                  0.097   Jarque-Bera (JB):                4.098
Skew:                           0.481   Prob(JB):                        0.129
Kurtosis:                       3.243   Cond. No.                         1.74
==============================================================================
Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
```

The parameter names here have been given the generic names x1, x2, and so on. Suppose instead that all of the model parameters are in a DataFrame:

```
In [74]: data = pd.DataFrame(X, columns=['col0', 'col1', 'col2'])

In [75]: data['y'] = y

In [76]: data[:5]
Out[76]:
       col0      col1      col2         y
```

```
0 -0.129468 -1.212753  0.504225  0.427863
1  0.302910 -0.435742 -0.254180 -0.673480
2 -0.328522 -0.025302  0.138351 -0.090878
3 -0.351475 -0.719605 -0.258215 -0.489494
4  1.243269 -0.373799 -0.522629 -0.128941
```

Now we can use the statsmodels formula API and Patsy formula strings:

```
In [77]: results = smf.ols('y ~ col0 + col1 + col2', data=data).fit()

In [78]: results.params
Out[78]:
Intercept    0.033559
col0         0.176149
col1         0.224826
col2         0.514808
dtype: float64

In [79]: results.tvalues
Out[79]:
Intercept    0.952188
col0         3.319754
col1         4.850730
col2         6.303971
dtype: float64
```

Observe how statsmodels has returned results as Series with the DataFrame column names attached. We also do not need to use `add_constant` when using formulas and pandas objects.

Given new out-of-sample data, you can compute predicted values given the estimated model parameters:

```
In [80]: results.predict(data[:5])
Out[80]:
0   -0.002327
1   -0.141904
2    0.041226
3   -0.323070
4   -0.100535
dtype: float64
```

There are many additional tools for analysis, diagnostics, and visualization of linear model results in statsmodels that you can explore. There are also other kinds of linear models beyond ordinary least squares.

Estimating Time Series Processes

Another class of models in statsmodels are for time series analysis. Among these are autoregressive processes, Kalman filtering and other state space models, and multivariate autoregressive models.

Let's simulate some time series data with an autoregressive structure and noise:

```
init_x = 4

import random
values = [init_x, init_x]
N = 1000

b0 = 0.8
b1 = -0.4
noise = dnorm(0, 0.1, N)
for i in range(N):
    new_x = values[-1] * b0 + values[-2] * b1 + noise[i]
    values.append(new_x)
```

This data has an AR(2) structure (two *lags*) with parameters 0.8 and –0.4. When you fit an AR model, you may not know the number of lagged terms to include, so you can fit the model with some larger number of lags:

```
In [82]: MAXLAGS = 5

In [83]: model = sm.tsa.AR(values)

In [84]: results = model.fit(MAXLAGS)
```

The estimated parameters in the results have the intercept first and the estimates for the first two lags next:

```
In [85]: results.params
Out[85]: array([-0.0062,  0.7845, -0.4085, -0.0136,  0.015 ,  0.0143])
```

Deeper details of these models and how to interpret their results is beyond what I can cover in this book, but there's plenty more to discover in the statsmodels documentation.

13.4 Introduction to scikit-learn

scikit-learn is one of the most widely used and trusted general-purpose Python machine learning toolkits. It contains a broad selection of standard supervised and unsupervised machine learning methods with tools for model selection and evaluation, data transformation, data loading, and model persistence. These models can be used for classification, clustering, prediction, and other common tasks.

There are excellent online and printed resources for learning about machine learning and how to apply libraries like scikit-learn and TensorFlow to solve real-world problems. In this section, I will give a brief flavor of the scikit-learn API style.

At the time of this writing, scikit-learn does not have deep pandas integration, though there are some add-on third-party packages that are still in development. pandas can be very useful for massaging datasets prior to model fitting, though.