Linear regression

Based on Python Data Science Handbook

Linear regression models are a good starting point for regression tasks. Such models are popular because they can be fit very quickly, and are very interpretable. You are probably familiar with the simplest form of a linear regression model (i.e., fitting a straight line to data) but such models can be extended to model more complicated data behavior.

In this section we will start with a quick intuitive walk-through of the mathematics behind this well-known problem, before seeing how before moving on to see how linear models can be generalized to account for more complicated patterns in data.

We begin with the standard imports:

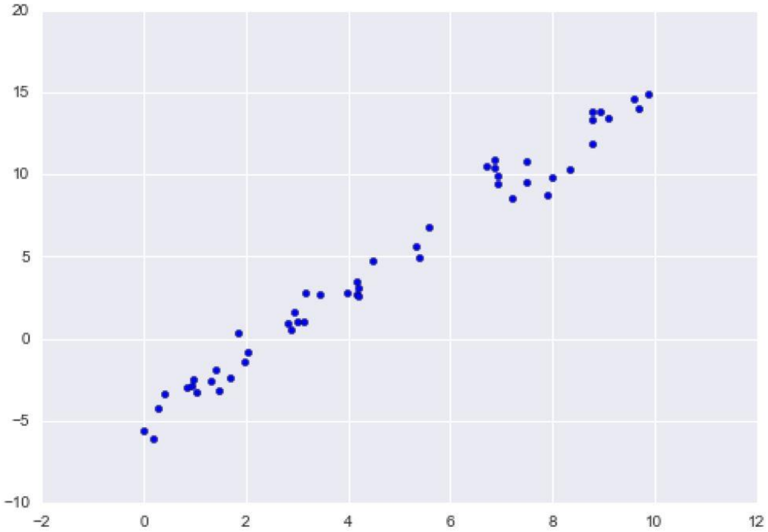
```
import matplotlib.pyplot as plt

import seaborn as sns; sns.set()

import numpy as np
```

Simple Linear Regression

We will start with the most familiar linear regression, a straight-line fit to data. A straight-line fit is a model of the form y = ax + b where a is known as the slope, and b is known as the intercept.

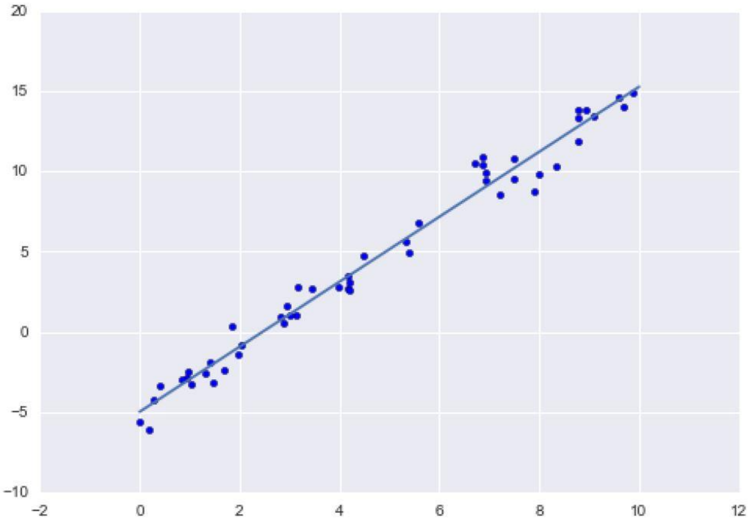
Consider the following data, which is scattered about a line with a slope of 2 and an intercept of -5

```
rng = np.random.RandomState(1)

x = 10 * rng.rand(50)

y = 2 * x - 5 + rng.randn(50)

plt.scatter(x, y)

plt.show()
```



We can use Scikit-Learn's LinearRegression estimator to fit this data and construct the best-fit line:

```
from sklearn.linear_model import LinearRegression
model = LinearRegression(fit_intercept=True)
model.fit(x[:, np.newaxis], y)

xfit = np.linspace(0, 10, 1000)
yfit = model.predict(xfit[:, np.newaxis])

plt.scatter(x, y)
plt.plot(xfit, yfit)
plt.show()
```



The slope and intercept of the data are contained in the model's fit parameters, which in Scikit-Learn are always marked by a trailing underscore. Here the relevant parameters are coef_ and intercept_

```
print("Model slope: ", model.coef_[0])

print("Model intercept:", model.intercept_)
```

```
Model slope: 2.02720881036

Model intercept: -4.99857708555
```

We see that the results are very close to the inputs, as we might hope.

The LinearRegression estimator is much more capable than this, however—in addition to simple straight-line fits, it can also handle multidimensional linear models of the form

$$y = a_0 + a_1 x_1 + a_2 x_2 + \cdots$$

where there are multiple x values. Geometrically, this is akin to fitting a plane to points in three dimensions, or fitting a hyper-plane to points in higher dimensions.

The multidimensional nature of such regressions makes them more difficult to visualize, but we can see one of these fits in action by building some example data, using NumPy's matrix multiplication operator:

```
rng = np.random.RandomState(1)

X = 10 * rng.rand(100, 3)

y = 0.5 + np.dot(X, [1.5, -2., 1.])

model.fit(X, y)

print(model.intercept_)

print(model.coef_)
```

```
0.5

[ 1.5 -2. 1. ]
```

Here the y data is constructed from three random x values, and the linear regression recovers the coeficients used to construct the data.

In this way, we can use the single LinearRegression estimator to fit lines, planes, or hyperplanes to our data. It still appears that this approach would be limited to strictly linear relationships between variables, but it turns out we can relax this as well.

Basis Functions

One trick you can use to adapt linear regression to nonlinear relationships between variables is to transform the data according to basis functions. The idea is to take our multidimensional linear model:

$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3 + \cdots$$

and build the x_1, x_2, x_3 and so on from our single-dimensional input x. Basically we let x_n=f_n(x) where f_n(x) is some function that transforms our data

$$y = a_0 + a_1f_1(x)+ a_2f_2(x) + a_3f_3(x) + \cdots$$

For example, if $f_n(x)=x^n$ then our model becomes a polynomial regression:

$$y = a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots$$

Notice that this is still a linear model—the linearity refers to the fact that the coefficients never multiply or divide each other. Essentially, we have taken our one-dimensional x-values and projected them into a higher dimension, so that a linear fit can can be found that fits more complex relationships between x and y.

Polynomial basis functions

The polynomial projection is built into Scikit-Learn using the PolynomialFeatures transformer:

```
from sklearn.preprocessing import PolynomialFeatures

x = np.array([2, 3, 4])

poly = PolynomialFeatures(3, include_bias=False)

poly.fit_transform(x[:, None])
```

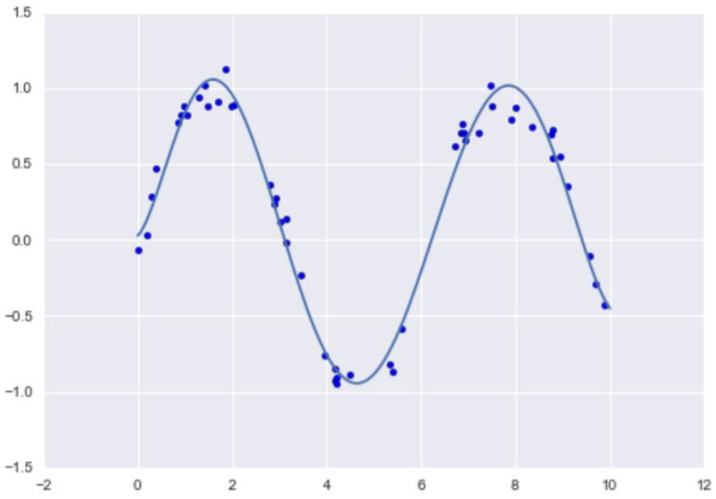
```
array([[ 2., 4., 8.],
       [ 3., 9., 27.],
       [ 4., 16., 64.]])
```

We see here that the transformer has converted our one-dimensional array into a three dimensional array by taking the exponent of each value. This new, higher-dimensional data representation can then be plugged into a linear regression. The cleanest way to accomplish this is to use a pipeline. Let's make a 7th-degree polynomial model in this way:

```
from sklearn.pipeline import make_pipeline

poly_model = make_pipeline(PolynomialFeatures(7),LinearRegression())
```

With this transform in place, we can use the linear model to fit more complex relationships between x and y. For example, here is a sin wave with noise:

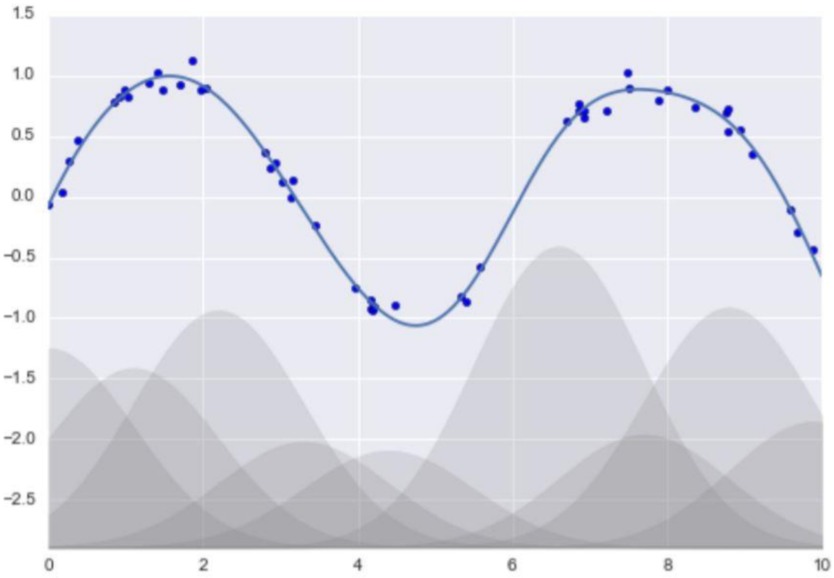
```
rng = np.random.RandomState(1)

x = 10 * rng.rand(50)

y = np.sin(x) + 0.1 * rng.randn(50)

xfit = np.linspace(0, 10, 1000)

poly_model.fit(x[:, np.newaxis], y)

yfit = poly_model.predict(xfit[:, np.newaxis])

plt.scatter(x, y)

plt.plot(xfit, yfit)

plt.show()
```



Our linear model, through the use of 7th-order polynomial basis functions, can provide an excellent fit to this non-linear data!

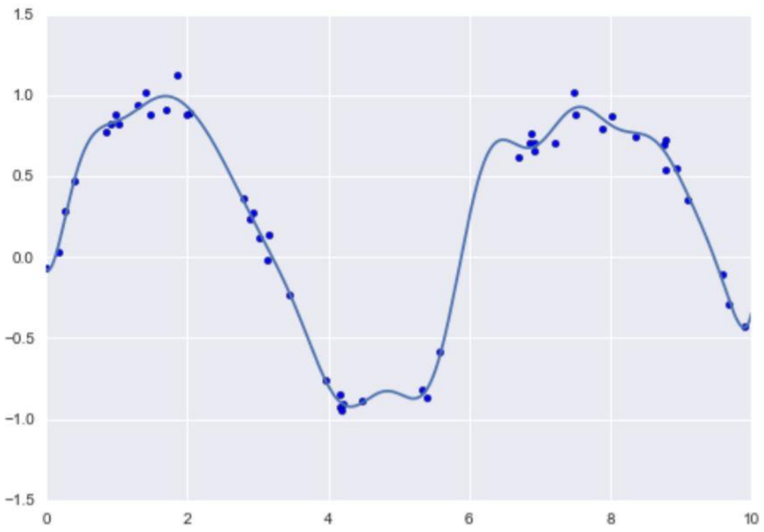
Gaussian basis functions

Other basis functions are possible. For example, one useful pattern is to fit a model that is not a sum of polynomial bases, but a sum of Gaussian bases. The result might look something like the following figure:



The shaded regions in the plot are the scaled basis functions, and when added together they reproduce the smooth curve through the data. These Gaussian basis functions are not built into Scikit-Learn, but we can write a custom transformer that will create them, as shown here and illustrated in the following figure (Scikit-Learn transformers are implemented as Python classes; reading Scikit-Learn's source is a good way to see how they can be created):

```
from sklearn.base import BaseEstimator, TransformerMixin

class GaussianFeatures(BaseEstimator, TransformerMixin):
   """Uniformly spaced Gaussian features for one-dimensional input"""

   def __init__(self, N, width_factor=2.0):
      self.N = N
      self.width_factor = width_factor

   @staticmethod
   def _gauss_basis(x, y, width, axis=None):
      arg = (x - y) / width
      return np.exp(-0.5 * np.sum(arg ** 2, axis))

   def fit(self, X, y=None):
      # create N centers spread along the data range
      self.centers_ = np.linspace(X.min(), X.max(), self.N)
      self.width_ = self.width_factor * (self.centers_[1] - self.centers_[0])
      return self

   def transform(self, X):
      return self._gauss_basis(X[:, :, np.newaxis], self.centers_, self.width_, axis=1)

gauss_model = make_pipeline(GaussianFeatures(20),LinearRegression())
gauss_model.fit(x[:, np.newaxis], y)
yfit = gauss_model.predict(xfit[:, np.newaxis])

plt.scatter(x, y)
plt.plot(xfit, yfit)
plt.xlim(0, 10)
plt.show()
```

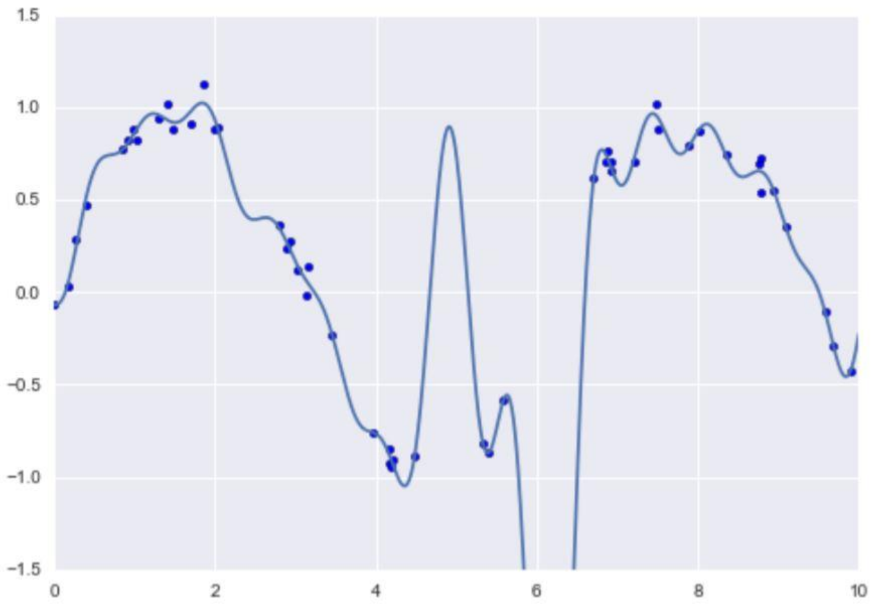


We put this example here just to make clear that there is nothing magic about polynomial basis functions: if you have some sort of intuition into the generating process of your data that makes you think one basis or another might be appropriate, you can use them as well.

Regularization

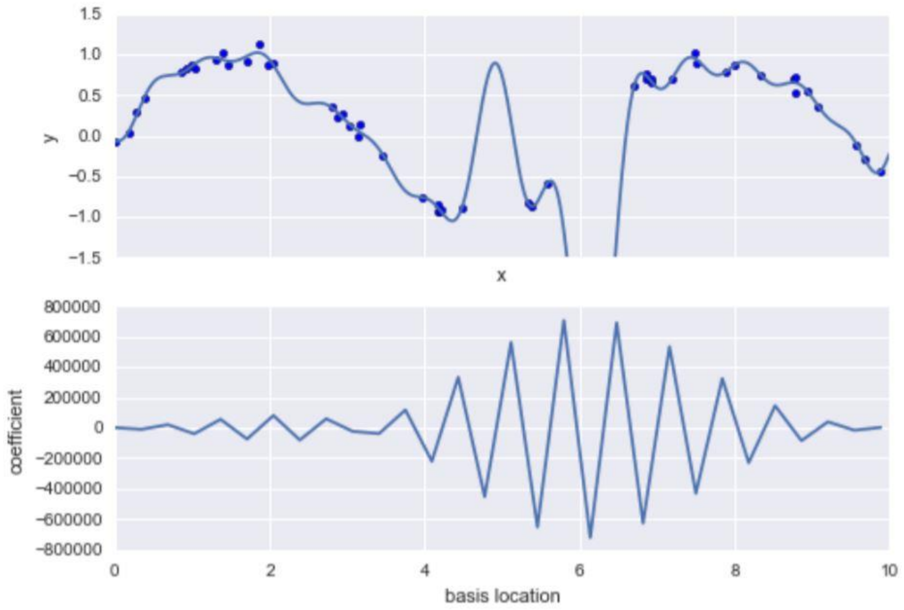
The introduction of basis functions into our linear regression makes the model much more flexible, but it also can very quickly lead to overfitting. For example, if we choose too many Gaussian basis functions, we end up with results that don't look so good:

```
model = make_pipeline(GaussianFeatures(30), LinearRegression())

model.fit(x[:, np.newaxis], y)

plt.scatter(x, y)

plt.plot(xfit, model.predict(xfit[:, np.newaxis]))

plt.xlim(0, 10)

plt.ylim(-1.5,  1.5)
```



With the data projected to the 30-dimensional basis, the model has far too much flexibility and goes to extreme values between locations where it is constrained by data. We can see the reason for this if we plot the coeficients of the Gaussian bases with respect to their locations:

```
def basis_plot(model, title=None):
    fig, ax = plt.subplots(2, sharex=True)
    model.fit(x[:, np.newaxis], y)
    ax[0].scatter(x, y)
    ax[0].plot(xfit, model.predict(xfit[:, np.newaxis]))
    ax[0].set(xlabel='x', ylabel='y', ylim=(-1.5, 1.5))

    if title:
        ax[0].set_title(title)
    ax[1].plot(model.steps[0][1].centers_, model.steps[1][1].coef_)
    ax[1].set(xlabel='basis location', ylabel='coefficient', xlim=(0, 10))
    plt.show()

model = make_pipeline(GaussianFeatures(30), LinearRegression())
basis_plot(model)
```



The lower panel of this figure shows the amplitude of the basis function at each location. This is typical overfitting behavior when basis functions overlap: the coeicients of adjacent basis functions blow up and cancel each other out. We know that such behavior is problematic, and it would be nice if we could limit such spikes expliticly in the model by penalizing large values of the model parameters. Such a penalty is known as regularization, and comes in several forms.

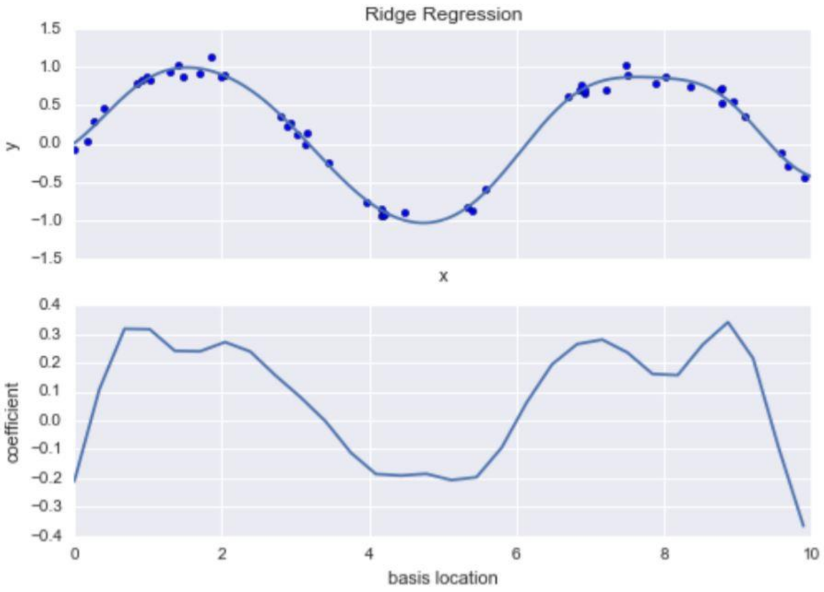
Ridge regression (L2 Regularization)

Perhaps the most common form of regularization is known as Ridge regression or L2 regularization. This proceeds by penalizing the sum of squares (2-norms) of the model regression coefficients; in this case, the penalty on the model fit is:

$$P = \alpha \sum_{n=1}^{N} \theta_n^2$$

where α is a free parameter that controls the strength of the penalty. This type of penalized model is built into Scikit-Learn with the Ridge estimator:

```
from sklearn.linear_model import Ridge

model = make_pipeline(GaussianFeatures(30), Ridge(alpha=0.1))

basis_plot(model, title='Ridge Regression')
```



The α parameter essentially controls the complexity of the resulting model. In the limit α→0, we recover the standard linear regression result; in the limit α→∞ , all model responses will be suppressed. One advantage of ridge regression in particular is that it can be computed very efficiently; no more computational cost than the original linear regression model.

Lasso regression (L1 regularization)

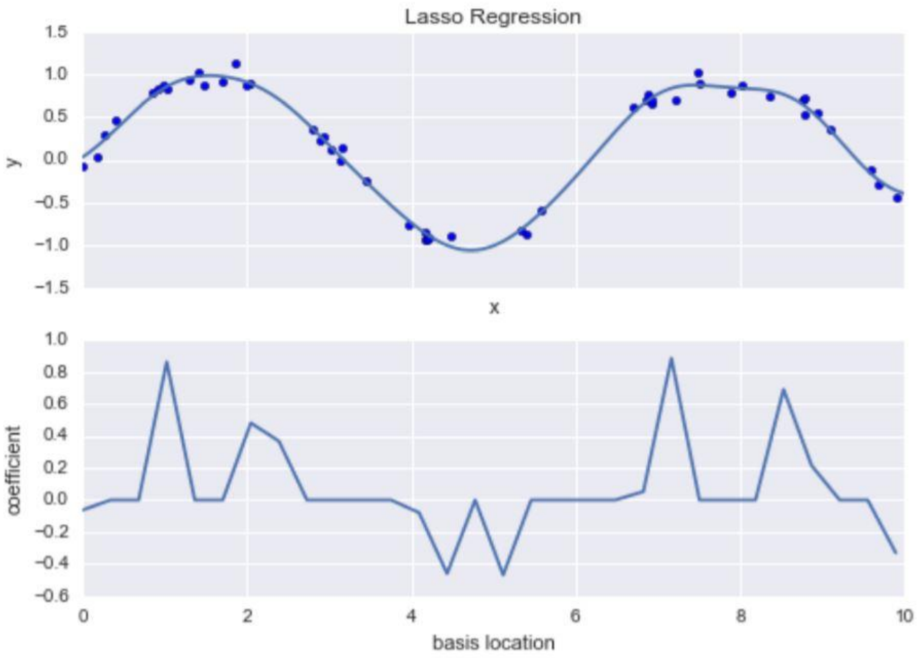
Another very common type of regularization is known as Lasso regression. It involves penalizing the sum of absolute values (1-norms) of the regression coeficients:

$$P = \alpha \sum_{n=1}^{N} |\,\theta_n|$$

Though this is conceptually very similar to Ridge regression, the results can differ surprisingly: for example, due to geometric reasons Lasso regression tends to favor sparse models where possible: that is, it preferentially sets model coefficients to exactly zero.

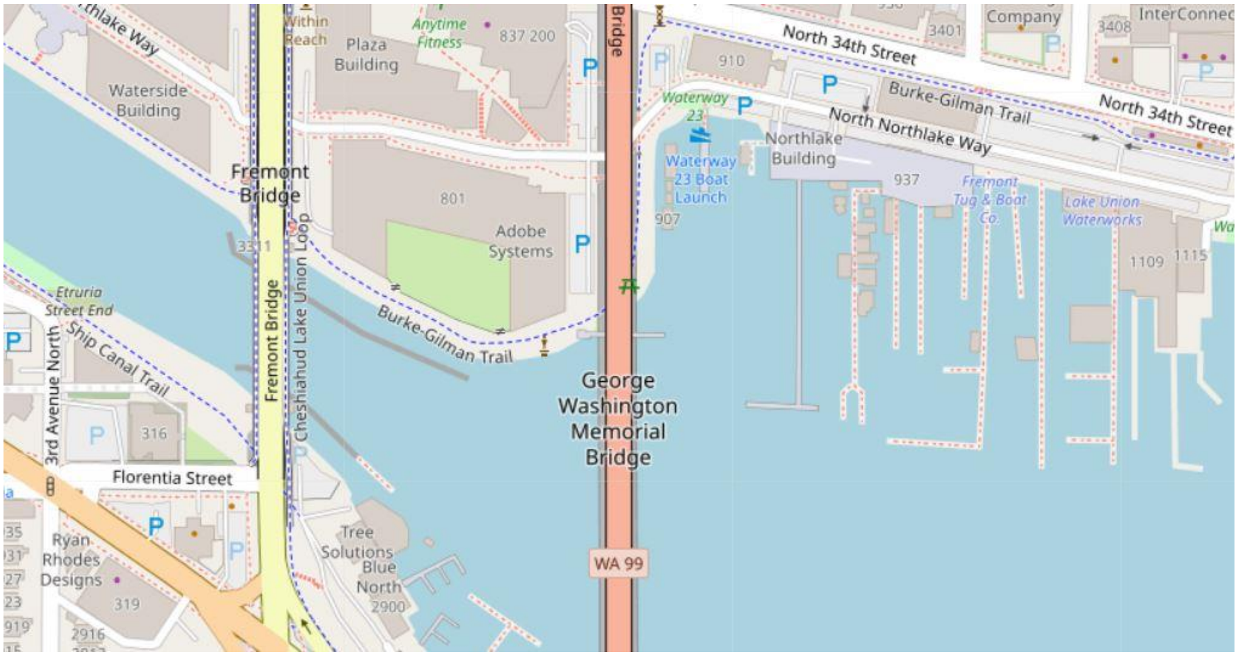
We can see this behavior in duplicating the Ridge regression figure, but using L1-normalized coefficients:

```
from sklearn.linear_model import Lasso

model = make_pipeline(GaussianFeatures(30), Lasso(alpha=0.001))

basis_plot(model, title='Lasso Regression')
```



With the Lasso regression penalty, the majority of the coefficients are exactly zero, with the functional behavior being modeled by a small subset of the available basis functions. As with Ridge regularization, the α parameter tunes the strength of the penalty, and it should be determined via cross-validation.

Case Study: Predicting Bicycle Traffic (OPTIONAL PART)



As an example, let's take a look at whether we can predict the number of bicycle trips across Seattle's Fremont Bridge based on weather, season, and other factors.

In this section, we will join the bike data with another dataset, and try to determine the extent to which weather and seasonal factors—temperature, precipitation, and daylight hours—affect the volume of bicycle traffic through this corridor.

The National Centers for Environmental Information (NOAA) makes available their daily weather station data (http://www.ncdc.noaa.gov/cdo-web/search?datasetid=GHCND). The Seattle Department of Transportation makes available the Fremont bike counters at http://www.seattle.gov/transportation/projects-and-programs/programs/bike-program/bike-counters/fremont-bike-counters

We can easily use Pandas to join the two data sources. We will perform a simple linear regression to relate weather and other information to bicycle counts, in order to estimate how a change in any one of these parameters affects the number of riders on a given day.

In particular, this is an example of how the tools of Scikit-Learn can be used in a statistical modeling framework, in which the parameters of the model are assumed to have interpretable meaning. This is not a standard approach within machine learning, but such interpretation is possible for some models.

Let's start by downloading the two datasets FremontBridge.csv and BicycleWeather.csv from the course website. Then, we can load the two datasets in Python by indexing them by date:

```
import pandas as pd

counts = pd.read_csv('FremontBridge.csv', index_col='Date', parse_dates=True)

weather = pd.read_csv('BicycleWeather.csv', index_col='DATE', parse_dates=True)
```

Next we will compute the total daily bicycle traffic, and put this in its own dataframe:

```
daily = counts.resample('d').sum()

daily['Total'] = daily.sum(axis=1)

daily = daily[['Total']] # remove other columns
```

We saw previously that the patterns of use generally vary from day to day; let's account for this in our data by adding binary columns that indicate the day of the week:

```
days = ['Mon', 'Tue', 'Wed', 'Thu', 'Fri', 'Sat', 'Sun']
for i in range(7):
    daily[days[i]] = (daily.index.dayofweek == i).astype(float)
```

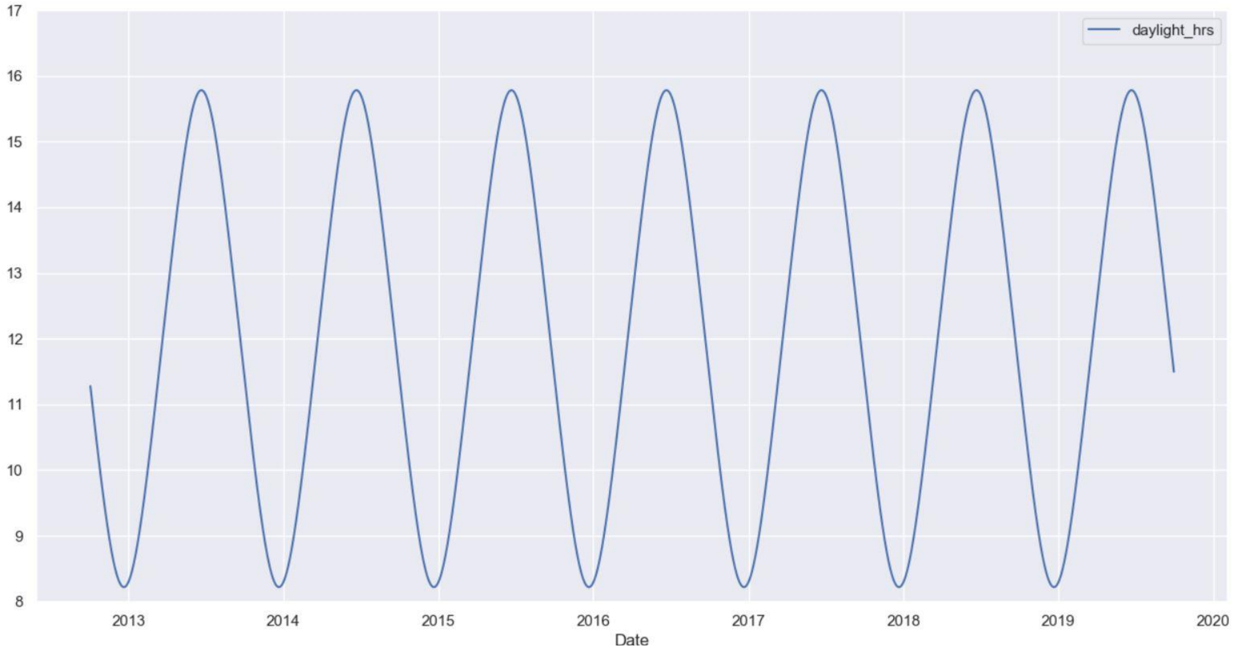
Similarly, we might expect riders to behave differently on holidays; let’s add an indicator of this as well:

```
from pandas.tseries.holiday import USFederalHolidayCalendar

cal = USFederalHolidayCalendar()

holidays = cal.holidays('2012', '2016')

daily = daily.join(pd.Series(1, index=holidays, name='holiday'))

daily['holiday'].fillna(0, inplace=True)
```

We also might suspect that the hours of daylight would affect how many people ride; let's use the standard astronomical calculation to add this information:

```
def hours_of_daylight(date, axis=23.44, latitude=47.61):
    """Compute the hours of daylight for the given date"""
    days = (date - pd.datetime(2000, 12, 21)).days
    m = (1. - np.tan(np.radians(latitude))* np.tan(np.radians(axis) * np.cos(days * 2 * np.pi / 365.25)))
    return 24. * np.degrees(np.arccos(1 - np.clip(m, 0, 2))) / 180.

daily['daylight_hrs'] = list(map(hours_of_daylight, daily.index))
daily[['daylight_hrs']].plot()
plt.ylim(8, 17)
plt.show()
```

```
(8, 17)
```



We can also add the average temperature and total precipitation to the data. In addition to the inches of precipitation, let's add a flag that indicates whether a day is dry (has zero precipitation):

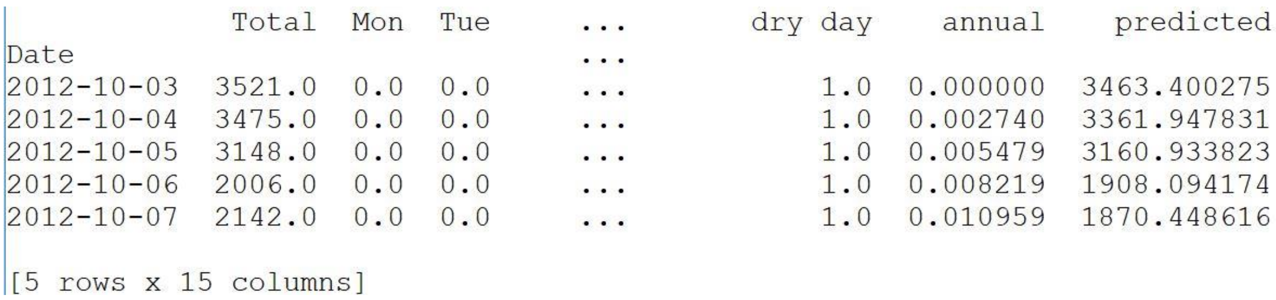
```
# temperatures are in 1/10 deg C; convert to C

weather['TMIN'] /= 10

weather['TMAX'] /= 10

weather['Temp (C)'] = 0.5 * (weather['TMIN'] + weather['TMAX'])

# precip is in 1/10 mm; convert to inches

weather['PRCP'] /= 254

weather['dry day'] = (weather['PRCP'] == 0).astype(int)

daily = daily.join(weather[['PRCP', 'Temp (C)', 'dry day']])
```

Finally, let's add a counter that increases from day 1, and measures how many years have passed. This will let us measure any observed annual increase or decrease in daily crossings:

```
daily['annual']  = (daily.index - daily.index[0]).days / 365.
```

Now our data is in order, and we can take a look at it:

```
daily.head()
```



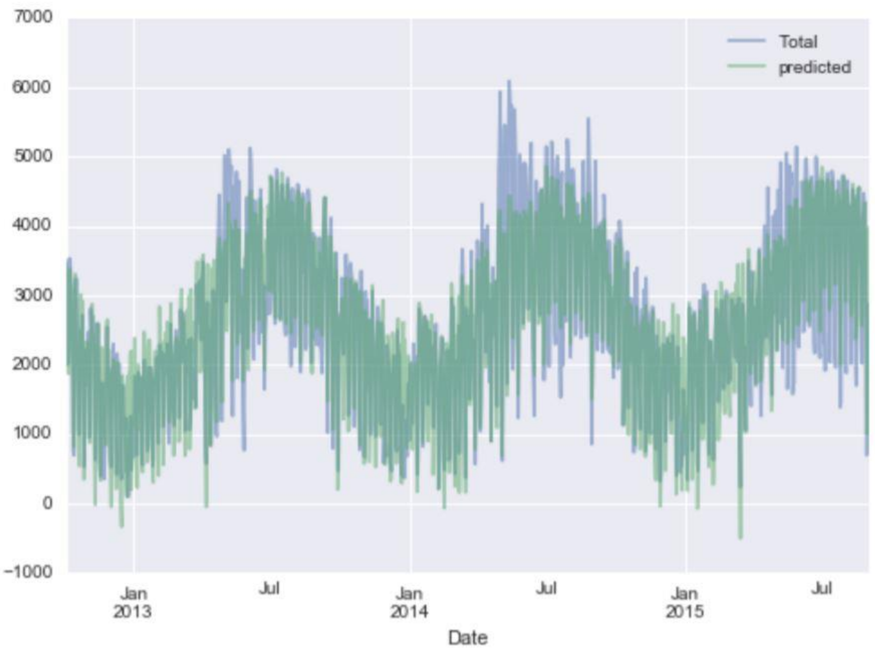
```
             Total  Mon  Tue     ...       dry day    annual    predicted
Date                             ...
2012-10-03  3521.0  0.0  0.0     ...           1.0  0.000000  3463.400275
2012-10-04  3475.0  0.0  0.0     ...           1.0  0.002740  3361.947831
2012-10-05  3148.0  0.0  0.0     ...           1.0  0.005479  3160.933823
2012-10-06  2006.0  0.0  0.0     ...           1.0  0.008219  1908.094174
2012-10-07  2142.0  0.0  0.0     ...           1.0  0.010959  1870.448616

[5 rows x 15 columns]
```

With this in place, we can choose the columns to use, and fit a linear regression model to our data. We will set fit_intercept = False , because the daily flags essentially operate as their own day-specific intercepts:

```
# Drop any rows with null values
daily.dropna(axis=0, how='any', inplace=True)
column_names   =   ['Mon','Tue','Wed','Thu','Fri','Sat','Sun','holiday','daylight_hrs',
'PRCP','dry day','Temp (C)','annual']
X = daily[column_names]
y = daily['Total']
model = LinearRegression(fit_intercept=False)
model.fit(X, y)
daily['predicted'] = model.predict(X)
```

Finally, we can compare the total and predicted bicycle traffic visually:

```
daily[['Total', 'predicted']].plot(alpha=0.5)
plt.show()
```



It is evident that we have missed some key features, especially during the summer time. Either our features are not complete (i.e., people decide whether to ride to work based on more than just these) or there are some nonlinear relationships that we have failed to take into account (e.g., perhaps people ride less at both high and low temperatures). Nevertheless, our rough approximation is enough to give us some insights, and we can take a look at the coefficients of the linear model to estimate how much each feature contributes to the daily bicycle count:

```
params = pd.Series(model.coef_, index=X.columns)
params
```

```
Mon                    504.882756
Tue                    610.233936
Wed                    592.673642
Thu                    482.358115
Fri                    177.980345
Sat                  -1103.301710
Sun                  -1133.567246
holiday              -1187.401381
daylight_hrs           128.851511
PRCP                  -664.834882
dry day                547.698592
Temp (C)                65.162791
annual                  26.942713
dtype: float64
```

These numbers are difficult to interpret without some measure of their uncertainty. We can compute these uncertainties quickly using bootstrap resamplings of the data:

```
from sklearn.utils import resample

np.random.seed(1)

err = np.std([model.fit(*resample(X, y)).coef_ for i in range(1000)], 0)
```

With these errors estimated, let's again look at the results:

```
print(pd.DataFrame({'effect': params.round(0), 'error': err.round(0)}))
```

```
                effect       error
Mon              505.0       86.0
Tue              610.0       83.0
Wed              593.0       83.0
Thu              482.0       85.0
Fri              178.0       81.0
Sat            -1103.0       80.0
Sun            -1134.0       83.0
holiday        -1187.0       163.0
daylight_hrs     129.0       9.0
PRCP            -665.0       62.0
dry day          548.0       33.0
Temp (C)          65.0       4.0
annual            27.0       18.0
```

We first see that there is a relatively stable trend in the weekly baseline: there are many more riders on weekdays than on weekends and holidays. We see that for each additional hour of daylight, 129 ± 9 more people choose to ride; a temperature increase of one degree Celsius encourages 65 ± 4 people to grab their bicycle; a dry day means an average of 548 ± 33 more riders, and each inch of precipitation means 665 ± 62 more people leave their bike at home. Once all these effects are accounted for, we see a modest increase of 27 ± 18 new daily riders each year.

Our model is almost certainly missing some relevant information. For example, nonlinear effects (such as effects of precipitation and cold temperature) and nonlinear trends within each variable (such as disinclination to ride at very cold and very hot temperatures) cannot be accounted for in this model. Additionally, we have thrown away some of the finer-grained information (such as the difference between a rainy morning and a rainy afternoon), and we have ignored correlations between days (such as the possible effect of a rainy Tuesday on Wednesday's numbers, or the effect of an unexpected sunny day after a streak of rainy days). These are all potentially interesting effects, and you now have the tools to begin exploring them if you wish!