A Python Companion to ISLR

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1 Introduction

1 Introduction

Figure 1 shows graphs of Wage versus three variables.

Figure 2 shows boxplots of previous days' percentage changes in S&P 500 grouped according to today's change $\tt Up$ or $\tt Down.$

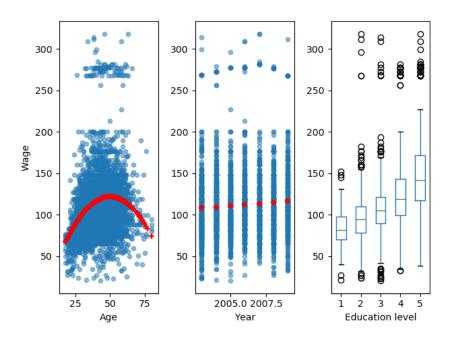


Figure 1: Wage data, which contains income survey information for males from the central Atlantic region of the United States. Left: wage as a function of age. On average, wage increases with age until about 60 years of age, at which point it begins to decline. Center: wage as a function of year. There is a slow but steady increase of approximately \$10,000 in the average wage between 2003 and 2009. Right: Boxplots displaying wage as a function of education, with 1 indicating the lowest level (no highschool diploma) and 5 the highest level (an advanced graduate degree). On average, wage increases with the level of education.

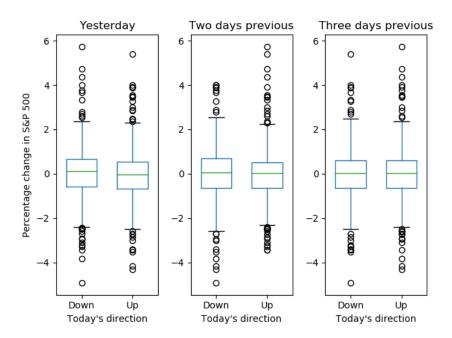


Figure 2: Left: Boxplots of the previous day's percentage change in the S&P 500 index for the days for which the market increased or decreased, obtained from the Smarket data. Center and Right: Same as left panel, but the percentage changes for two and three days previous are shown.

2 Statistical Learning

2.1 What is Statistical Learning?

Figure 3 shows scatter plots of sales versus TV, radio, and newspaper advertising. In each panel, the figure also includes an OLS regression line.

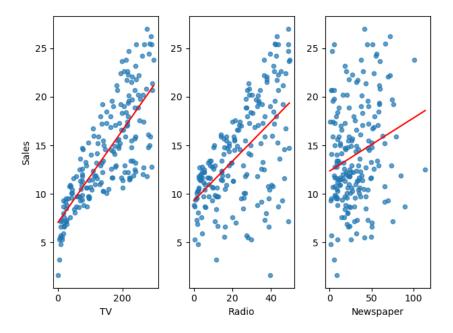


Figure 3: The Advertising data set. The plot displays sales, in thousands of units, as a function of TV, radio, and newspaper budgets, in thousands of dollars, for 200 different markets. In each plot we show the simple least squares fit of sales to that variable. In other words, each red line represents a simple model that can be used to predict sales using TV, radio, and newspaper, respectively.

Figure 4 is a plot of Income versus Years of Education from the Income data set. In the left panel, the "true" function (given by blue line) is actually my guess.

Figure 5 is a plot of Income versus Years of Education and Seniority from the Income data set. Since the book does not provide the true values of Income, "true" values shown in the plot are actually third order polynomial fit.

Figure 6 shows an example of the parametric approach applied to the

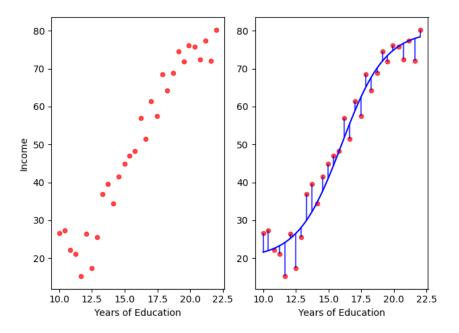


Figure 4: The Income data set. Left: The red dots are the observed values of income (in tens of thousands of dollars) and years of education for 30 individuals. Right: The blue curve represents the true underlying relationship between income and years of education, which is generally unknown (but is known in this case because the data are simulated). The vertical lines represent the error associated with each observation. Note that some of the errors are positive (when an observation lies above the blue curve) and some are negative (when an observation lies below the curve). Overall, these errors have approximately mean zero.

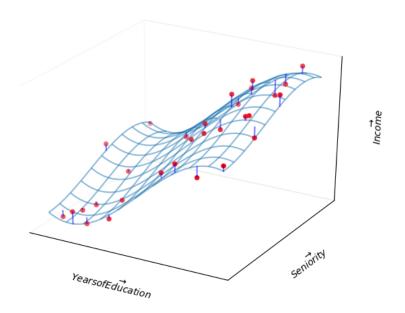


Figure 5: The plot displays income as a function of years of education and seniority in the Income data set. The blue surface represents the true underlying relationship between income and years of education and seniority, which is known since the data are simulated. The red dots indicate the observed values of these quantities for 30 individuals.

Income data from previous figure.

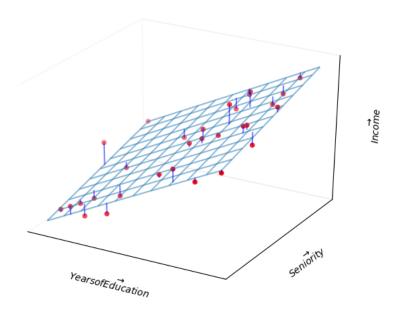


Figure 6: A linear model fit by least squares to the Income data from figure 5. The observations are shown in red, and the blue plane indicates the least squares fit to the data.

Figure 7 provides an illustration of the trade-off between flexibility and interpretability for some of the methods covered in this book.

Figure 8 provides a simple illustration of the clustering problem.

2.2 Assessing Model Accuracy

Figure 9 illustrates the tradeoff between training MSE and test MSE. We select a "true function" whose shape is similar to that shown in the book. In the left panel, the orange, blue, and green curves illustrate three possible estimates for f given by the black curve. The orange line is the linear regression fit, which is relatively inflexible. The blue and green curves were produced using $smoothing\ splines$ from UnivariateSpline function in scipy package. We obtain different levels of flexibility by varying the parameter s, which affects the number of knots.

For the right panel, we have chosen polynomial fits. The degree of polynomial represents the level of flexibility. This is because the function

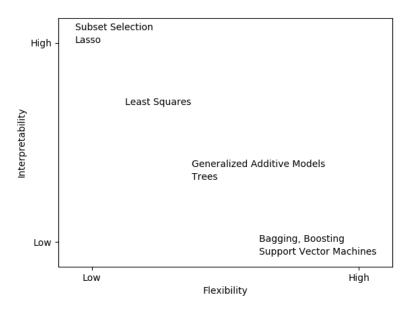


Figure 7: A representation of the tradeoff between flexibility and interpretability, using different statistical learning methods. In general, as the flexibility of a method increases, its interpretability decreases.

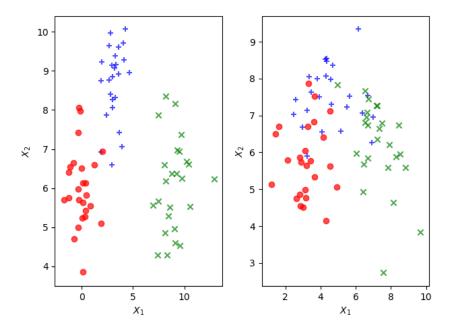


Figure 8: A clustering data set involving three groups. Each group is shown using a different colored symbol. Left: The three groups are well-separated. In this setting, a clustering approach should successfully identify the three groups. Right: There is some overlap among the groups. Now the clustering taks is more challenging.

UnivariateSpline does not more than five degrees of freedom.

When we repeat the simulations for figure 9, we see considerable variation in the right panel MSE plots. But the overall conclusion remains the same.

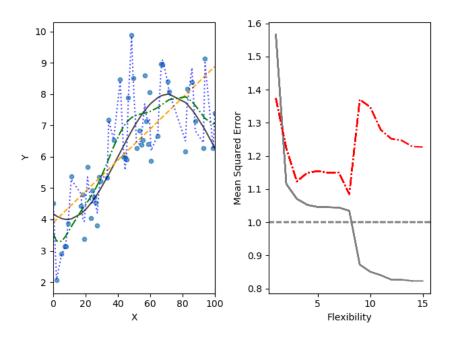


Figure 9: Left: Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two smoothing spline fits (blue and green curves). Right: Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed grey line).

Figure 10 provides another example in which the true f is approximately linear.

Figure 11 displays an example in which f is highly non-linear. The training and test MSE curves still exhibit the same general patterns.

Figure 12 displays the relationship between bias, variance, and test MSE. This relationship is referred to as bias-variance trade-off. When simulations are repeated, we see considerable variation in different graphs, especially for MSE lines. But overall shape remains the same.

Figure 13 provides an example using a simulated data set in two-dimensional space consisting of predictors X_1 and X_2 .

Figure 14 displays the KNN decision boundary, using K = 10, when

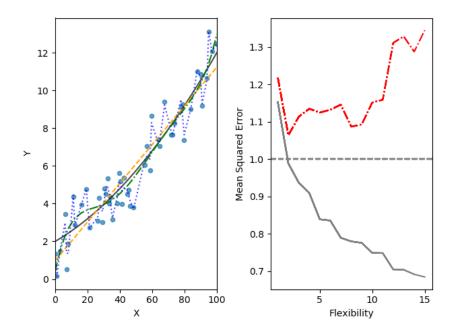


Figure 10: Details are as in figure 9 using a different true f that is much closer to linear. In this setting, linear regression provides a very good fit to the data.

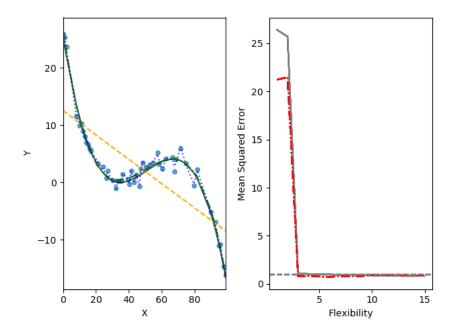


Figure 11: Details are as in figure 9, using a different f that is far from linear. In this setting, linear regression provides a very poor fit to the data.

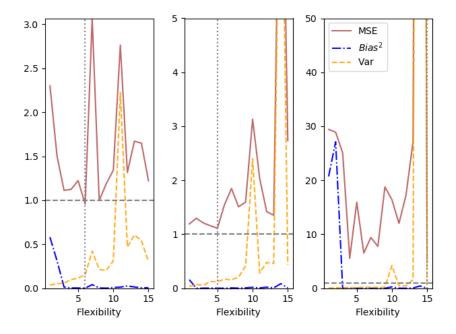


Figure 12: Squared bias (blue curve), variance (orange curve), $Var(\epsilon)$ (dashed line), and test MSE (red curve) for the three data sets in figures 9 - 11. The vertical dotted line indicates the flexibility level corresponding to the smallest test MSE.

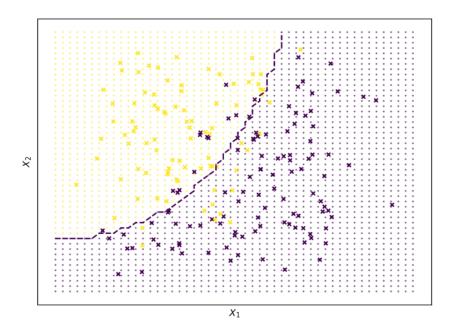


Figure 13: A simulated data set consisting of 200 observations in two groups, indicated in blue and orange. The dashed line represents the Bayes decision boundary. The orange background grid indicates the region in which a test observation will be assigned to the orange class, and blue background grid indicates the region in which a test observation will be assigned to the blue class.

applied to the simulated data set from figure 13. Even though the true distribution is not known by the KNN classifier, the KNN decision making boundary is very close to that of the Bayes classifier.

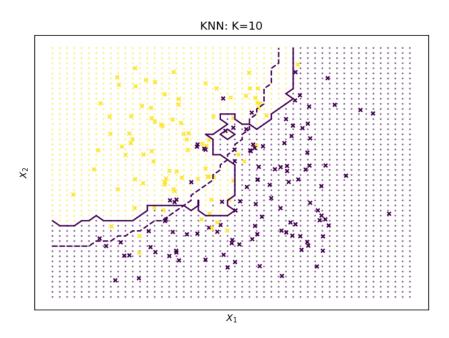


Figure 14: The firm line indicates the KNN decision boundary on the data from figure 13, using K=10. The Bayes decision boundary is shown as a dashed line. The KNN and Bayes decision boundaries are very similar.

In figure 16 we have plotted the KNN test and training errors as a function of $\frac{1}{K}$. As $\frac{1}{K}$ increases, the method becomes more flexible. As in the regression setting, the training error rate consistently declines as the flexibility increases. However, the test error exhibits the characteristic U-shape, declining at first (with a minimum at approximately K=10) before increasing again when the method becomes excessively flexible and overfits.

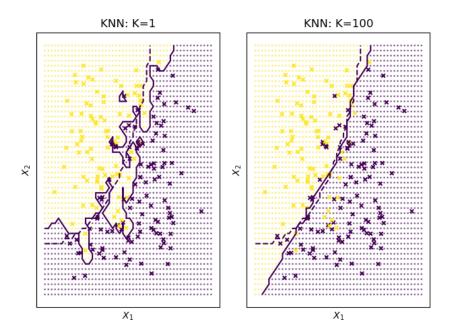


Figure 15: A comparison of the KNN decision boundaries (solid curves) obtained using K=1 and K=100 on the data from figure 13. With K=1, the decision boundary is overly flexible, while with K=100 it is not sufficiently flexible. The Bayes decision boundary is shown as dashed line.

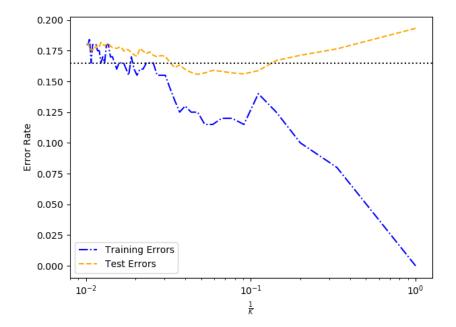


Figure 16: The KNN training error rate (blue, 200 observations) and test error rate (orange, 5,000 observations) on the data from figure 13 as the level of flexibility (assessed using $\frac{1}{K}$) increases, or equivalently as the number of neighbors K decreases. The black dashed line indicates the Bayes error rate.

2.3 Lab: Introduction to Python

2.3.1 Basic Commands

In Python a list can be created by enclosing comma-separated elements by square brackets. Length of a list can be obtained using len function.

```
x = [1, 3, 2, 5]
print(len(x))
y = 3
z = 5
print(y + z)
4
8
```

To create an array of numbers, use array function in numpy library. numpy functions can be used to perform element-wise operations on arrays.

```
import numpy as np
x = np.array([[1, 2], [3, 4]])
y = np.array([6, 7, 8, 9]).reshape((2, 2))
print(x)
print(y)
print(x ** 2)
print(np.sqrt(y))
[[1 2]
 [3 4]]
[[6 7]
 [8 9]]
[[1 4]
 [ 9 16]]
[[2.44948974 2.64575131]
 [2.82842712 3.
                        ]]
```

<code>numpy.random</code> has a number of functions to generate random variables that follow a given distribution. Here we create two correlated sets of numbers, x and y, and use <code>numpy.corrcoef</code> to calculate correlation between them.

```
import numpy as np
np.random.seed(911)
x = np.random.normal(size=50)
y = x + np.random.normal(loc=50, scale=0.1, size=50)
print(np.corrcoef(x, y))
print(np.corrcoef(x, y)[0, 1])
print(np.mean(x))
print(np.var(y))
print(np.std(y) ** 2)
             0.99374931]
 [0.99374931 1.
                       ]]
0.9937493134584551
-0.020219724397254404
0.9330621750073689
0.9330621750073688
```

2.3.2 Graphics

matplotlib library has a number of functions to plot data in Python. It is possible to view graphs on screen or save them in file for inclusion in a document.

numpy function linspace can be used to create a sequence between a start and an end of a given length.

```
import numpy as np
```

```
import matplotlib.pyplot as plt

x = np.linspace(-np.pi, np.pi, num=50)
y = x
xx, yy = np.meshgrid(x, y)
zz = np.cos(yy) / (1 + xx ** 2)

plt.contour(xx, yy, zz)

fig, ax = plt.subplots()
zza = (zz - zz.T) / 2.0
CS = ax.contour(xx, yy, zza)
ax.clabel(CS, inline=1)
```

2.3.3 Indexing Data

To access elements of an array, specify indexes inside square brackets. It is possible to access multiple rows and columns. shape method gives number of rows followed by number of columns.

```
import numpy as np
A = np.array(np.arange(1, 17))
A = A.reshape(4, 4, order='F') # column first, Fortran style
print(A)
print(A[1, 2])
print(A[(0,2),:][:,(1,3)])
print(A[range(0,3),:][:,range(1,4)])
print(A[range(0, 2), :])
print(A[:, range(0, 2)])
print(A[0,:])
print(A.shape)
[[ 1 5 9 13]
 [ 2 6 10 14]
 [ 3 7 11 15]
 [ 4 8 12 16]]
10
[ 5 15]
[ 5 10 15]
[[ 1 5 9 13]
```

```
[ 2 6 10 14]]
[[1 5]
[2 6]
[3 7]
[4 8]]
(4, 4)
```

2.3.4 Loading Data

pandas library provides read_csv function to read files with data in rectangular shape.

```
import pandas as pd
Auto = pd.read_csv('data/Auto.csv')
print(Auto.head())
print(Auto.shape)
print(Auto.columns)
```

```
mpg cylinders displacement
                                           origin
                                 ... year
                                                                        name
0 18.0
                          307.0
                                       70
                                                1 chevrolet chevelle malibu
                8
1 15.0
                8
                          350.0
                                       70
                                                           buick skylark 320
2 18.0
                8
                          318.0 ...
                                       70
                                                1
                                                          plymouth satellite
3 16.0
                8
                          304.0
                                       70
                                                               amc rebel sst
                                 . . .
                                                1
4 17.0
                          302.0 ...
                                       70
                                                1
                                                                 ford torino
```

To load data from an R library, use get_rdataset function from statsmodels. This function seems to work only if the computer is connected to the internet.

2.3.5 Additional Graphical and Numerical Summaries

plot method can be directly applied to a pandas dataframe.

```
import pandas as pd
Auto = pd.read_csv('data/Auto.csv')
Auto.boxplot(column='mpg', by='cylinders', grid=False)
```

hist method can be applied to plot a histogram.

```
import pandas as pd
Auto = pd.read_csv('data/Auto.csv')
Auto.hist(column='mpg')
Auto.hist(column='mpg', color='red')
Auto.hist(column='mpg', color='red', bins=15)
```

For pairs plot, use scatter_matrix method in pandas.plotting.

On pandas dataframes, describe method produces a summary of each variable.

```
import pandas as pd
Auto = pd.read_csv('data/Auto.csv')
print(Auto.describe())
```

	mpg	cylinders	 year	origin
count	397.000000	397.000000	 397.000000	397.000000
mean	23.515869	5.458438	 75.994962	1.574307
std	7.825804	1.701577	 3.690005	0.802549
min	9.000000	3.000000	 70.000000	1.000000
25%	17.500000	4.000000	 73.000000	1.000000
50%	23.000000	4.000000	 76.000000	1.000000
75%	29.000000	8.000000	 79.000000	2.000000
max	46.600000	8.000000	 82.000000	3.000000

[8 rows x 7 columns]

3 Linear Regression

3.1 Simple Linear Regression

Figure 17 displays the simple linear regression fit to the Advertising data, where $\hat{\beta_0} = 0.0475$ and $\hat{\beta_1} = 7.0326$.

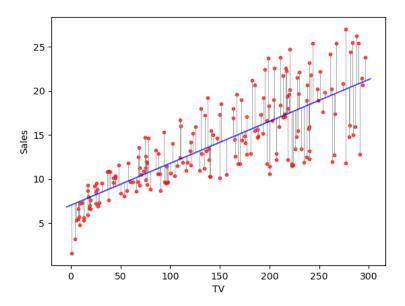


Figure 17: For the Advertising data, the least squares fit for the regression of sales onto TV is shown. The fit is found by minimizing the sum of squared errors. Each grey line represents an error, and the fit makes a compromise by averaging their squares. In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.

In figure 18, we have computed RSS for a number of values of β_0 and β_1 , using the advertising data with sales as the response and TV as the predictor.

The left-hand panel of figure 19 displays population regression line and least squares line for a simple simulated example. The red line in the left-hand panel displays the true relationship, f(X) = 2 + 3X, while the blue line is the least squares estimate based on observed data. In the right-hand panel of figure 19 we have generated five different data sets from the model $Y = 2 + 3X + \epsilon$ and plotted the corresponding five least squares lines.

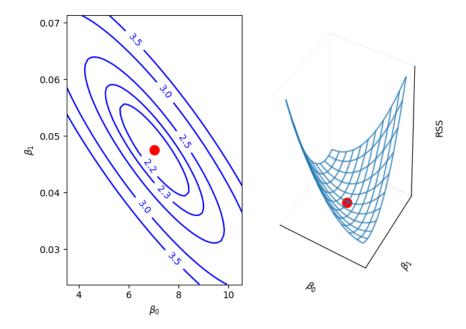


Figure 18: Contour and three-dimensional plots of the RSS on the Advertising data, using sales as the response and TV as the predictor. The red dots correspond to the least squares estimates $\hat{\beta_0}$ and $\hat{\beta_1}$.

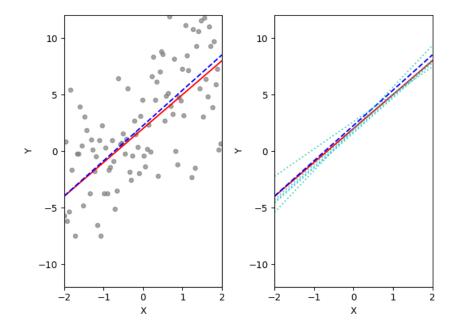


Figure 19: A simulated data set. Left: The red line represents the true relationship, f(X) = 2 + 3X, which is known as the population regression line. The blue line is the least squares line; it is the least squares estimate for f(X) based on the observed data, shown in grey circles. Right: The population regression line is again shown in red, and the least squares line in blue. In cyan, five least squares lines are shown, each computed on the basis of a separate random set of observations. Each least squares line is different, but on average, the least squares lines are quite close to the population regression line.

For Advertising data, table 1 provides details of the least squares model for the regression of number of units sold on TV advertising budget.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	7.0326	0.4578	15.3603	0.0
TV	0.0475	0.0027	17.6676	0.0

Table 1: For Advertising data, the coefficients of the least squares model for the regression of number of units sold on TV advertising budget. An increase of \$1,000 on the TV advertising budget is associated with an increase in sales by around 50 units.

Next, in table 2, we report more information about the least squares model.

Quantity	Value
Residual standard error	3.259
R^2	0.612
F-statistic	312.145

Table 2: For the Advertising data, more information about the least squares model for the regression of number of units sold on TV advertising budget.

3.2 Multiple Linear Regression

Table 3 shows results of two simple linear regressions, each of which uses a different advertising medium as a predictor. We find that a \$1,000 increase in spending on radio advertising is associated with an increase in sales by around 202 units. A \$1,000 increase in advertising spending on on newspapers increases sales by approximately 55 units.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	9.312	0.563	16.542	0.0
radio	0.202	0.02	9.921	0.0
Intercept	12.351	0.621	19.876	0.0
newspaper	0.055	0.017	3.3	0.001

Table 3: More simple linear regression models for Advertising data. Coefficients of the simple linear regression model for number of units sold on Top: radio advertising budget and Bottom: newspaper advertising budget. A \$1,000 increase in spending on radio advertising is associated with an average increase sales by around 202 units, while the same increase in spending on newspaper advertising is associated with an average increase of around 55 units. Sales variable is in thousands of units, and the radio and newspaper variables are in thousands of dollars..

Figure 20 illustrates an example of the least squares fit to a toy data set with p=2 predictors.

Table 4 displays multiple regression coefficient estimates when TV, radio, and newspaper advertising budgets are used to predict product sales using Advertising data.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	2.939	0.312	9.422	0.0
TV	0.046	0.001	32.809	0.0
radio	0.189	0.009	21.893	0.0
newspaper	-0.001	0.006	-0.177	0.86

Table 4: For the Advertising data, least squares coefficient estimates of the multiple linear regression of number of units sold on radio, TV, and newspaper advertising budgets.

Table 5 shows the correlation matrix for the three predictor variables and response variable in table 4.

Figure 21 displays a three-dimensional plot of TV and radio versus sales.

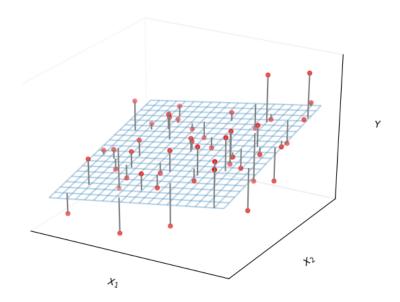


Figure 20: In a three-dimensional setting, with two predictors and one response, the least squares regression line becomes a plane. The plane is chosen to minimize the sum of the squared vertical distances between each observation (shown in red) and the plane.

	TV	radio	newspaper	$_{\mathrm{sales}}$
TV	1.0	0.0548	0.0566	0.7822
radio	0.0548	1.0	0.3541	0.5762
newspaper	0.0566	0.3541	1.0	0.2283
sales	0.7822	0.5762	0.2283	1.0

Table 5: Correlation matrix for TV, radio, and sales for the Advertising data.

Quantity	Value
Residual standard error	1.69
R^2	0.897
F-statistic	570.0

Table 6: More information about the least squares model for the regression of number of units sold on TV, newspaper, and radio advertising budgets in the Advertising data. Other information about this model was displayed in table 4.

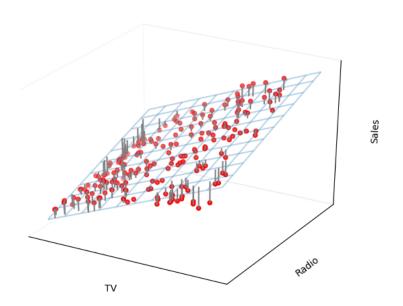


Figure 21: For the Advertising data, a linear regression fit to sales using TV and radio as predictors. From the pattern of the residuals, we can see that there is a pronounced non-linear relationship in the data. The positive residuals tend to lie along the 45-degree line, where TV and Radio budgets are split evenly. The negative residuals tend to lie away from this line, where budgets are more lopsided.

3.3 Other Considerations in the Regression Model

Credit data set displayed in figure 22 records balance (average credit card debt for a number of individuals) as well as several quantitative predictors: age, cards (number of credit cards), education and rating (credit rating).

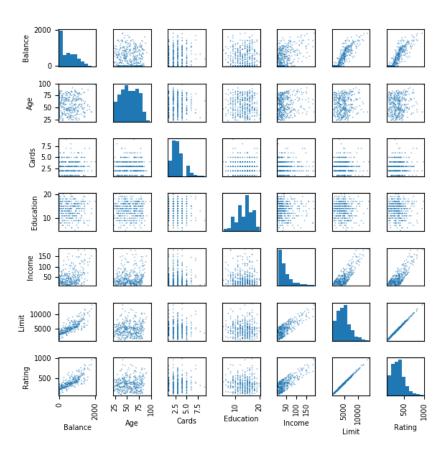


Figure 22: The Credit dataset contains information about balance, age, cards, education, income, limit, and rating for a number of potential customers.

Table 7 displays the coefficient estimates and other information associated with the model where gender is the only explanatory variable.

From table 8 we see that the estimated balance for the baseline, African American, is \$531.0. It is estimated that the Asian category will have an additional \$-18.7 debt, and that the Caucasian category will have an additional \$-12.5 debt compared to African American category.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	509.803	33.128	15.389	0.0
Gender[T.Female]	19.733	46.051	0.429	0.669

Table 7: Least squares coefficient estimates associated with the regression of balance onto gender in the Credit data set.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	531.0	46.319	11.464	0.0
Ethnicity[T.Asian]	-18.686	65.021	-0.287	0.774
Ethnicity[T.Caucasian]	-12.503	56.681	-0.221	0.826

Table 8: Least squares coefficient estimates associated with the regression of balance onto ethnicity in the Credit data set.

Table 9 shows results of regressing sales and TV and radio when an interaction term is included. Coefficient of interaction term TV:radio is highly significant.

In figure 23, the left panel shows least squares lines when we predict balance using income (quantitative) and student (qualitative variables). There is no interaction term between income and student. The right panel shows least squares lines when an interaction term is included.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	6.75	0.248	27.233	0.0
TV	0.019	0.002	12.699	0.0
radio	0.029	0.009	3.241	0.001
TV:radio	0.001	0.0	20.727	0.0

Table 9: For Advertising data, least squares coefficient estimates associated with the regression of sales onto TV and radio, with an interaction term.

Figure 24 shows a scatter plot of mpg (gas mileage in miles per gallon) versus horsepower in the Auto data set. The figure also includes least squares fit line for linear, second degree, and fifth degree polynomials in horsepower.

Table 10 shows regression results of a quadratic fit to explain mpg as a function of horsepower and $horsepower^2$.

The left panel of figure 25 displays a residual plot from the linear regression of mpg onto horsepower on the Auto data set. The red line is a smooth fit to the residuals, which is displayed in order to make it easier to identify

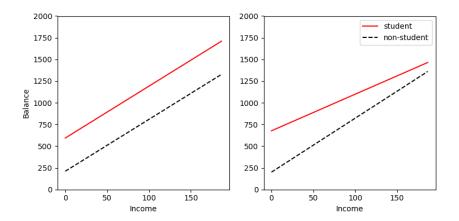


Figure 23: For the Credit data, the least squares lines are shown for prediction of balance from income for students and non-students. Left: There is no interaction between income and student. Right: There is an interaction term between income and students.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	56.9001	1.8004	31.6037	0.0
horsepower	-0.4662	0.0311	-14.9782	0.0
$horsepower^2$	0.0012	0.0001	10.0801	0.0

Table 10: For the Auto data set, least squares coefficient estimates associated with the regression of mpg onto horsepower and

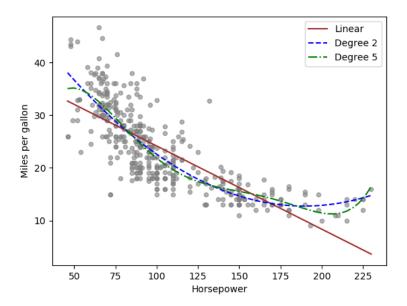


Figure 24: The Auto data set. For a number of cars, mpg and horsepower are shown. The linear regression fit is shown in orange. The linear regression fit for a model that includes first- and second-order terms of horsepower is shown as blue curve. The linear regression fit for a model that includes all polynomials of horsepower up to fifth-degree is shown in green.

any trends. The residuals exhibit a clear U-shape, which strongly suggests non-linearity in the data. In contrast, the right hand panel of figure 25 displays the residual plot results from the model which contains a quadratic term in horsepower. Now there is little pattern in residuals, suggesting that the quadratic term improves the fit to the data.

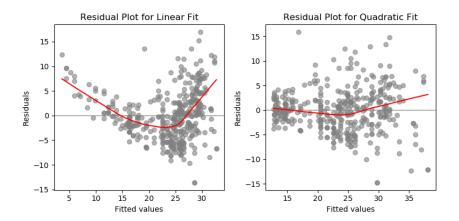


Figure 25: Plots of residuals versus predicted (or fitted) values for the Auto data set. In each plot, the red line is a smooth fit to the residuals, intended to make it easier to identify a trend. Left: A linear regression of mpg on horsepower. A strong pattern in the residuals indicates non-linearity in the data. Right: A linear regression of mpg on horsepower and square of horsepower. Now there is little pattern in the residuals.

Figure 26 provides an illustration of correlations among residuals. In the top panel, we see the residuals from a linear regression fit to data generated with uncorrelated errors. There is no evidence of time-related trend in the residuals. In contrast, the residuals in the bottom panel are from a data set in which adjacent errors had a correlation of 0.9. Now there is a clear pattern in the residuals - adjacent residuals tend to take on similar values. Finally, the center panel illustrates a more moderate case in which the residuals had a correlation of 0.5. There is still evidence of tracking, but the pattern is less pronounced.

In the left-hand panel of figure 27, the magnitude of the residuals tends to increase with the fitted values. The right hand panel displays residual plot after transforming the response using $\log(Y)$. The residuals now appear to have constant variance, although there is some evidence of a non-linear relationship in the data.

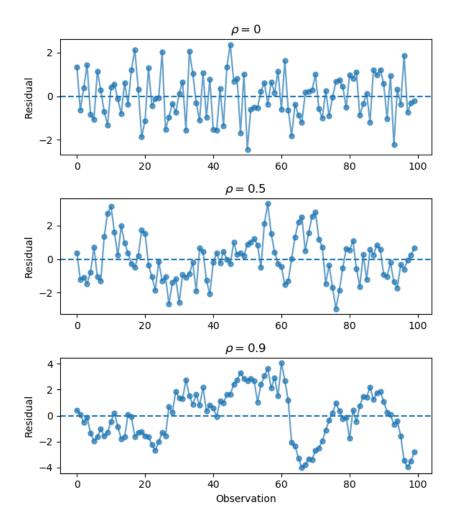


Figure 26: Plots of residuals from simulated time series data sets generated with differeing levels of correlation ρ between error terms for adjacent time points.

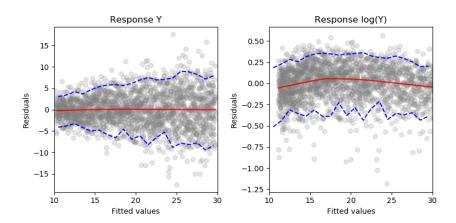


Figure 27: Residual plots. The red line, a smooth fit to the residuals, is intended to make it easier to identify a trend. The blue lines track 5^{th} and 95^{th} percentiles of the residuals, and emphasize patterns. Left: The funnel shape indicates heteroscedasticity. Right: the response has been log transformed, and now there is no evidence of heteroscedasticity.

The red point (observation 20) in the left hand panel of figure 28 illustrates a typical outlier. The red solid line is the least squares regression fit, while the blue dashed line is the least squares fit after removal of the outlier. In this case, removal of outlier has little effect on the least squares line. In the center panel of figure 28, the outlier is clearly visible. In practice, to decide if the outlier is sufficiently big to be considered an outlier, we can plot studentized residuals, computed by dividing each residual ϵ_i by its estimated standard error. These are shown in the right hand panel.

Observation 41 in the left-hand panel in figure 29 has high leverage, in that the predictor value for this observation is large relative to the other observations. The data displayed in figure 29 are the same as the data displayed in figure 28, except for the addition of a single high leverage observation¹. The red solid line is the least squares fit to the data, while the blue dashed line is the fit produced when observation 41 is removed. Comparing the left-hand panels of figures 28 and 29, we observe that removing the high leverage observation has a much more substantial impact on least squares line than removing the outlier. The center panel of figure 29, for a data set with two predictors X_1 and X_2 . While most of the observations' predictor values fall within the region of blue dashed lines, the red observation is well outside this

¹The middle panel is from a different data set.

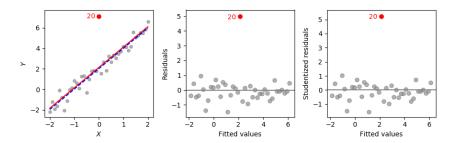


Figure 28: Left: The least squares regression line is shown in red. The regression line after removing the outlier is is shown in blue. Center: The residual plot clearly identifies the outlier. Right: The outlier has a studentized residual of 6; typically we expect values between -3 and 3.

range. But neither the value for X_1 nor the value for X_2 is unusual. So if we examine just X_1 or X_2 , we will not notice this high leverage point. The right-panel of figure 29 provides a plot of studentized residuals versus h_i for the data in the left hand panel. Observation 41 stands out as having a very high leverage statistic as well as a high studentized residual.

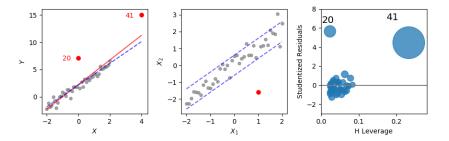


Figure 29: Left: Observation 41 is a high leverage point, while 20 is not. The red line is the fit to all the data, and the blue line is the fit with observation 41 removed. Center: The red observation is not unusual in terms of its X_1 value or its X_2 value, but still falls outside the bulk of the data, and hence has high leverage. Right: Observation 41 has a high leverage and a high residual.

Figure 30 illustrates the concept of collinearity.

Figure 31 illustrates some of the difficulties that can result from collinearity. The left panel is a contour plot of the RSS associated with different possible coefficient estimates for the regression of balance on limit and age.

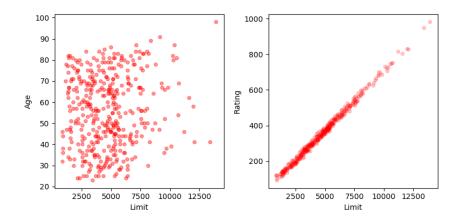


Figure 30: Scatter plots of the observations from the Credit data set. Left: A plot of age versus limit. These two variables not collinear. Right: A plot of rating versus limit. There is high collinearity.

Each ellipse represents a set of coefficients that correspond to the same RSS, with ellipses nearest to the center taking on the lowest values of RSS. The black dot and the associated dashed lines represent the coefficient estimates that result in the smallest possible RSS. The axes for limit and age have been scaled so that the plot includes possible coefficients that are up to four standard errors on either side of the least squares estimates. We see that the true limit coefficient is almost certainly between 0.15 and 0.20.

In contrast, the right hand panel of figure 31 displays contour plots of the RSS associated with possible coefficient estimates for the regression of balance onto limit and rating, which we know to be highly collinear. Now the contours run along a narrow valley; there is a broad range of values for the coefficient estimates that result in equal values for RSS.

Table 11 compares the coefficient estimates obtained from two separate multiple regression models. The first is a regression of balance on age and limit. The second is a regression of balance on rating and limit. In the first regression, both age and limit are highly significant with very small p-values. In the second, the collinearity between limit and rating has caused the standard error for the limit coefficient to increase by a factor of 12 and the p-value to increase to 0.701. In other words, the importance of the limit variable has been masked due to the presence of collinearity.

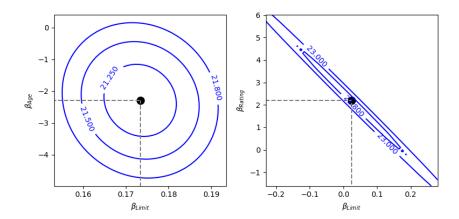


Figure 31: Contour plots for the RSS values as a function of the parameters β for various regressions involving the Credit data set. In each plot, the black dots represent the coefficient values corresponding to the minimum RSS. Left: A contour plot of RSS for the regression of balance onto age and limit. The minimum value is well defined. Right: A contour plot of RSS for the regression of balance onto rating and limit. Because of the collinearity, there are many pairs $(\beta_{Limit}, \beta_{Rating})$ with a similar value for RSS.

	Coef.	Std.Err.	t	$P > \mid t \mid$
Intercept	-173.411	43.828	-3.957	0.0
Age	-2.291	0.672	-3.407	0.001
Limit	0.173	0.005	34.496	0.0
Intercept	-377.537	45.254	-8.343	0.0
Rating	2.202	0.952	2.312	0.021
Limit	0.025	0.064	0.384	0.701

Table 11: The results for two multiple regression models involving the Credit data set. The top panel is a regression of balance on age and limit. The bottom panel is a regression of balance on rating and limit. The standard error of $\hat{\beta}_{Limit}$ increases 12-fold in the second regression, due to collinearity.

3.4 The Marketing Plan

3.5 Comparison of Linear Regression with K-Nearest Neighbors

Figure 32 illustrates two KNN fits on a data set with p=2 predictors. The fit with K=1 is shown in the left-hand panel, while the right-hand panel displays the fit with K=9. When K=1, the KNN fit perfectly interpolates the training observations, and consequently takes the form of a step function. When K=9, the KNN fit is still a step function, but averaging over nine observations results in much smaller regions of constant prediction, and consequently a smoother fit.

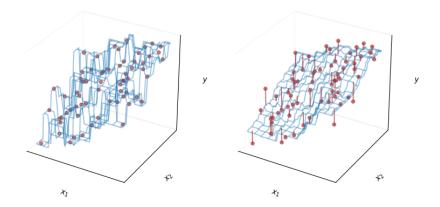


Figure 32: Plots of $\hat{f}(X)$ using KNN regression on two-dimensional data set with 64 observations (brown dots). Left: K = 1 results in a rough step function fit. Right: K = 9 produces a much smoother fit.

Figure 33 provides an example of KNN regression with data generated from a one-dimensional regression model. the black dashed lines represent f(X), while the blue curves correspond to the KNN fits using K=1 and K=9. In this case, the K=1 predictions are far too variable, while the smoother K=9 fit is much closer to f(X).

Figure 34 represents the linear regression fit to the same data. It is almost perfect. The right hand panel of figure 34 reveals that linear regression outperforms KNN for this data. The green line, plotted as a function of $\frac{1}{K}$, represents the test set mean squared error (MSE) for KNN. The KNN errors are well above the horizontal dashed line, which is the test MSE for linear regression.

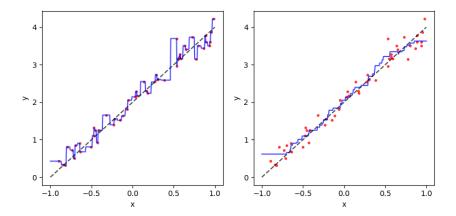


Figure 33: Plots of $\hat{f}(X)$ using KNN regression on a one-dimensional data set with 50 observations. The true relationship is given by the black dashed line. Left: The blue curve corresponds to K=1 and interpolates (i.e., passes directly through) training data. Right: The blue curve corresponds to K=9, and represents a smoother fit.

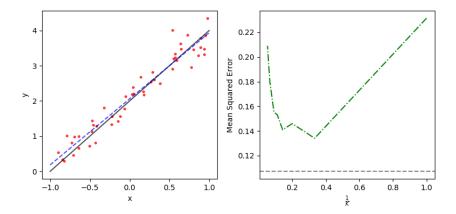


Figure 34: The same data set shown in figure 33 is investigated further. Left: The blue dashed line is the least squares fit to the data. Since f(X) is in fact linear (displayed in black line), the least squares regression line provides a very good estimate of f(X). Right: The dashed horizontal line represents the least squares test set MSE, while the green line corresponds to the MSE for KNN as a function of $\frac{1}{K}$. Linear regression achieves a lower test MSE than does KNN regression, since f(X) is in fact linear.

Figure 35 examines the relative performances of least squares regression and KNN under increasing levels of non-linearity in the relationship between X and Y. In the top row, the true relationship is nearly linear. In this case, we see that the test MSE for linear regression is still superior to that of KNN for low values of K (far right). However, as K increases, KNN outperforms linear regression. The second row illustrates a more substantial deviation from linearity. In this situation, KNN substantially outperforms linear regression for all values of K.

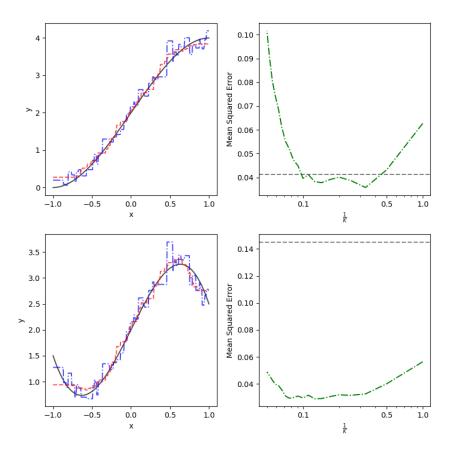


Figure 35: Top Left: In a setting with a slightly non-linear relationship between X and Y (solid black line), the KNN fits with K=1 (blue) and K=9 (red) are displayed. Top Right: For the slightly non-linear data,the test set MSE for least squares regression (horizontal) and KNN with various values of $\frac{1}{K}$ (green) are displayed. Bottom Left and Bottom Right: As in the top panel, but with a strongly non-linear relationship between X and Y.

Figure 36 considers the same strongly non-linear situation as in the lower panel of figure 35, except that we have added additional *noise* predictors that are not associated with the response. When p=1 or p=2, KNN outperforms linear regression. But as we increase p, linear regression becomes superior to KNN. In fact, increase in dimensionality has only caused a small increase in linear regression test set MSE, but it has caused a much bigger increase in the MSE for KNN.

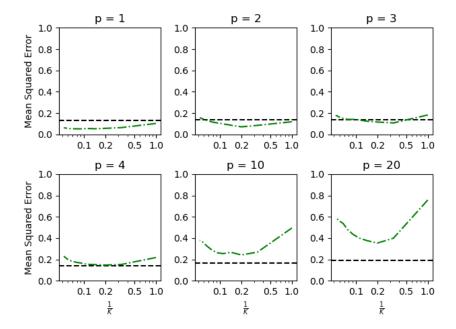


Figure 36: Test MSE for linear regressions (black horizontal lines) and KNN (green curves) as the number of variables p increases. The true function is non-linear in the first variable, as in the lower panel in figure 35, and does not depend upon the additional variables. The performance of linear regression deteriorates slowly in the presense of these additional variables, whereas KNN's performance degrades more quickly as p increases.

3.6 Lab: Linear Regression

3.6.1 Libraries

The import function, along with an optional as, is used to load *libraries*. Before a library can be loaded, it must be installed on the system.

```
import numpy as np
import statsmodels.formula.api as smf
```

3.6.2 Simple Linear Regression

No. Observations:

We load Boston data set from R library MASS. Then we use ols function from statsmodels.formula.api to fit simple linear regression model, with medv as response and lstat as the predictor.

Function summary2() gives some basic information about the model. We can use dir() to find out what other pieces of information are stored in lm_fit. The predict() function can be used to produce prediction of medv for a given value of lstat.

```
import statsmodels.formula.api as smf
from statsmodels import datasets
boston = datasets.get_rdataset('Boston', 'MASS').data
print(boston.columns)
print('----')
lm_reg = smf.ols(formula='medv ~ lstat', data=boston)
lm_fit = lm_reg.fit()
print(lm_fit.summary2())
print('----')
print(dir(lm_fit))
print('----')
print(lm_fit.predict(exog=dict(lstat=[5, 10, 15])))
Index(['crim', 'zn', 'indus', 'chas', 'nox', 'rm', 'age', 'dis', 'rad', 'tax',
      'ptratio', 'black', 'lstat', 'medv'],
     dtype='object')
               Results: Ordinary least squares
______
Model:
                  OLS
                                  Adj. R-squared:
                                                    0.543
Dependent Variable: medv
                                  AIC:
                                                    3286.9750
Date:
                  2019-05-28 14:10 BIC:
                                                    3295.4280
```

Log-Likelihood:

-1641.5

506

```
Df Model:
                 1
                                F-statistic:
                                                 601.6
                504
                               Prob (F-statistic): 5.08e-88
Df Residuals:
R-squared:
                0.544
                               Scale:
             Coef. Std.Err. t
                                   P>|t|
                                            [0.025 0.975]
______
           34.5538
                     0.5626 61.4151 0.0000 33.4485 35.6592
Intercept
                     0.0387 -24.5279 0.0000 -1.0261 -0.8740
lstat
           -0.9500
_____
                  137.043
                              Durbin-Watson:
Prob(Omnibus):
                  0.000
                              Jarque-Bera (JB):
                                                   291.373
Skew:
                  1.453
                              Prob(JB):
                                                   0.000
Kurtosis:
                  5.319
                              Condition No.:
                                                   30
_____
['HCO_se', 'HC1_se', 'HC2_se', 'HC3_se', '_HCCM', '__class__', '__delattr__',
'__dict__', '__dir__', '__doc__', '__eq__', '__format__', '__ge__',
'__getattribute__', '__gt__', '__hash__', '__init__', '__init_subclass__',
'__le__', '__lt__', '__module__', '__ne__', '__new__', '__reduce__',
'__reduce_ex__', '__repr__', '__setattr__', '__sizeof__', '__str__',
'__subclasshook__', '__weakref__', '_cache', '_data_attr',
'_get_robustcov_results', '_is_nested', '_wexog_singular_values', 'aic',
'bic', 'bse', 'centered_tss', 'compare_f_test', 'compare_lm_test',
'compare_lr_test', 'condition_number', 'conf_int', 'conf_int_el', 'cov_HCO',
'cov_HC1', 'cov_HC2', 'cov_HC3', 'cov_kwds', 'cov_params', 'cov_type',
'df_model', 'df_resid', 'eigenvals', 'el_test', 'ess', 'f_pvalue', 'f_test',
'fittedvalues', 'fvalue', 'get_influence', 'get_prediction',
'get_robustcov_results', 'initialize', 'k_constant', 'llf', 'load', 'model',
'mse_model', 'mse_resid', 'mse_total', 'nobs', 'normalized_cov_params',
'outlier_test', 'params', 'predict', 'pvalues', 'remove_data', 'resid',
'resid_pearson', 'rsquared', 'rsquared_adj', 'save', 'scale', 'ssr',
'summary', 'summary2', 't_test', 't_test_pairwise', 'tvalues',
'uncentered_tss', 'use_t', 'wald_test', 'wald_test_terms', 'wresid']
    29.803594
1
    25.053347
    20.303101
```

dtype: float64

We will now plot medv and 1stat along with least squares regression line.

```
import statsmodels.formula.api as smf
from statsmodels import datasets
boston = datasets.get_rdataset('Boston', 'MASS').data
print(boston.columns)
print('----')
lm_reg = smf.ols(formula='medv ~ lstat', data=boston)
lm_fit = lm_reg.fit()
print(lm_fit.summary2())
print('----')
print(dir(lm_fit))
print('----')
print(lm_fit.predict(exog=dict(lstat=[5, 10, 15])))
import statsmodels.api as sm
import matplotlib.pyplot as plt
fig = plt.figure()
ax = fig.add_subplot(111)
boston.plot(x='lstat', y='medv', alpha=0.7, ax=ax)
sm.graphics.abline_plot(model_results=lm_fit, ax=ax, c='r')
   Next we examine some diagnostic plots.
import statsmodels.formula.api as smf
from statsmodels import datasets
boston = datasets.get_rdataset('Boston', 'MASS').data
print(boston.columns)
print('----')
lm_reg = smf.ols(formula='medv ~ lstat', data=boston)
lm_fit = lm_reg.fit()
print(lm_fit.summary2())
print('----')
```

```
print(dir(lm_fit))
print('----')
print(lm_fit.predict(exog=dict(lstat=[5, 10, 15])))
import statsmodels.api as sm
from statsmodels.nonparametric.smoothers_lowess import lowess
import matplotlib.pyplot as plt
import numpy as np
fig = plt.figure()
ax1 = fig.add_subplot(221)
ax1.scatter(lm_fit.fittedvalues, lm_fit.resid, s=5, c='b', alpha=0.6)
ax1.axhline(y=0, linestyle='--', c='r')
# resid_lowess_fit = lowess(endog=lm_fit.resid, exog=lm_fit.fittedvalues,
#
                            is_sorted=True)
# ax1.plot(resid_lowess_fit[:,0], resid_lowess_fit[:,1])
ax1.set_xlabel('Fitted values')
ax1.set_ylabel('Residuals')
ax1.set_title('Residuals vs Fitted')
ax2=fig.add_subplot(222)
sm.graphics.qqplot(lm_fit.resid, ax=ax2, markersize=3, line='s',
   linestyle='--', fit=True, alpha=0.4)
ax2.set_ylabel('Standardized residuals')
ax2.set_title('Normal Q-Q')
influence = lm_fit.get_influence()
standardized_resid = influence.resid_studentized_internal
ax3 = fig.add_subplot(223)
ax3.scatter(lm_fit.fittedvalues, np.sqrt(np.abs(standardized_resid)), s=5,
    alpha=0.4, c='b')
ax3.set_xlabel('Fitted values')
ax3.set_ylabel(r'$\sqrt{\mid Standardized\; residuals \mid}$')
ax3.set_title('Scale-Location')
ax4 = fig.add_subplot(224)
sm.graphics.influence_plot(lm_fit, size=2, alpha=0.4, c='b', ax=ax4)
ax4.xaxis.label.set_size(10)
ax4.yaxis.label.set_size(10)
```

```
ax4.title.set_size(12)
ax4.set_xlim(0, 0.03)
for txt in ax4.texts:
    txt.set_visible(False)
ax4.axhline(y=0, linestyle='--', color='grey')
fig.tight_layout()
```

3.6.3 Multiple Linear Regression

In order to fit a multiple regression model using least squares, we again use the ols and fit functions. The syntax ols(formula='y $\sim x1 + x2 + x3$ ') is used to fit a model with three predictors, x1, x2, and x3. The summary2() now outputs the regression coefficients for all three predictors.

<code>statsmodels</code> does not seem to have R like facility to include all variables using the formula y $\tilde{}$... To include all variables, we either write them individually, or use code to create a formula.

```
import statsmodels.formula.api as smf
from statsmodels import datasets
boston = datasets.get_rdataset('Boston', 'MASS').data
lm_reg = smf.ols(formula='medv ~ lstat + age', data=boston)
lm_fit = lm_reg.fit()
print(lm_fit.summary2())
print('----')
# Create formula to include all variables
all_columns = list(boston.columns)
all_columns.remove('medv')
my_formula = 'medv ~ ' + ' + '.join(all_columns)
print(my_formula)
print('----')
all_reg = smf.ols(formula=my_formula, data=boston)
all_fit = all_reg.fit()
print(all_fit.summary2())
print('----')
```

Results:	Ordinary	least	squares
----------	----------	-------	---------

========	=======	========	.=======		:======	=======
Model: Dependent V		OLS medv	Ad AI	j. R-squar C:	red:	0.549 3281.0064
Date:		2019-05-29				3293.6860
No. Observa	ations:	506		g-Likeliho		-1637.5
Df Model:		2		statistic:		309.0
Df Residual				ob (F-stat		
R-squared:		0.551	Sc	ale: 		38.108
	Coef	. Std.Err	. t	P> t	[0.02	5 0.975]
Intercept	33.22	28 0.7308	3 45.45	79 0.0000	31.786	9 34.6586
lstat	-1.03	0.0482	2 -21.41	63 0.0000	-1.126	7 -0.9374
age	0.03	45 0.0122	2 2.82	56 0.0049	0.010	5 0.0586
Omnibus:		124.288	 Durb	in-Watson:		0.945
Prob(Omnibu	ıs):	0.000	Jarq	ue-Bera (J	ΙΒ):	244.026
Skew:		1.362	Prob	(JB):		0.000
Kurtosis:		5.038	Cond	ition No.:		201
medv ~ crimptratio + N		indus + chas stat	s + nox +	rm + age	+ dis +	rad + tax
	Re	sults: Ordin	nary leas	t squares		
Model:	======	======== OLS	 Ad	======= j. R-squar	:====== :ed:	0.734
Dependent V	Variable:	medv	AI	C:		3025.6086
Date:		2019-05-29	10:07 BI	C:		3084.7801
No. Observa	ations:	506	Lo	g-Likeliho	ood:	-1498.8
Df Model:		13	F-	statistic:		108.1
Df Residual		492		ob (F-stat		
R-squared:		0.741	Sc	ale:		22.518
	Coef.	Std.Err.	t	P> t	[0.025	0.975]
Intercept	36.4595	5.1035	7.1441	0.0000	26.4322	46.4868
crim	-0.1080	0.0329	-3.2865	0.0011	-0.1726	-0.0434

lstat	-0.5248 	0.0507	-10.3471	0.0000	-0.6244	-0.4251
black	0.0093	0.0027	3.4668	0.0006	0.0040	0.0146
ptratio	-0.9527	0.1308	-7.2825	0.0000	-1.2098	-0.6957
tax	-0.0123	0.0038	-3.2800	0.0011	-0.0197	-0.0049
rad	0.3060	0.0663	4.6129	0.0000	0.1757	0.4364
dis	-1.4756	0.1995	-7.3980	0.0000	-1.8675	-1.0837
age	0.0007	0.0132	0.0524	0.9582	-0.0253	0.0266
rm	3.8099	0.4179	9.1161	0.0000	2.9887	4.6310
nox	-17.7666	3.8197	-4.6513	0.0000	-25.2716	-10.2616
chas	2.6867	0.8616	3.1184	0.0019	0.9939	4.3796
indus	0.0206	0.0615	0.3343	0.7383	-0.1003	0.1414
zn	0.0464	0.0137	3.3816	0.0008	0.0194	0.0734

Omnibus: 178.041 Durbin-Watson: 1.078 Prob(Omnibus): 0.000 Jarque-Bera (JB): 783.126 Skew: Prob(JB): 1.521 0.000 Kurtosis: 8.281 Condition No.: 15114

narosete. Steel Sonaroton not.

3.6.4 Interaction Terms

The syntax lstat:black tells ols to include an interaction term between lstat and black. The syntax lstat*age simultaneously includes lstat, age, and the interaction term lstat×

```
import statsmodels.formula.api as smf
from statsmodels import datasets
```

boston = datasets.get_rdataset('Boston', 'MASS').data

```
my_reg = smf.ols(formula='medv ~ lstat * age', data=boston)
my_fit = my_reg.fit()
print(my_fit.summary2())
```

Results: Ordinary least squares

Model: OLS Adj. R-squared: 0.553
Dependent Variable: medv AIC: 3277.9547

^{*} The condition number is large (2e+04). This might indicate strong multicollinearity or other numerical problems.

Date: No. Observation Df Model: Df Residuals: R-squared:	ns: 50 3 50	2 556		Log-I F-sta Prob Scale	.ikelihoo atistic: (F-stati	od: .stic):	3294.8609 -1635.0 209.3 4.86e-88 37.804
	Coef.						5 0.975]
Intercept	36.0885	1.4698	3 24	. 5528	0.0000	33.200	7 38.9763
lstat	-1.3921	0.1675	5 -8	.3134	0.0000	-1.721	1 -1.0631
age	-0.0007	0.0199	9 -0	.0363	0.9711	-0.039	0.0383
lstat:age	0.0042	0.0019	9 2	. 2443	0.0252	0.000	5 0.0078
Omnibus:		35.601					0.965
Prob(Omnibus):		.000		-	Bera (JE	5):	296.955
Skew:		.417		rob(JE			0.000
Kurtosis:	ە ======	. 461 =======	Co =====	ond1t1 =====	lon No.:		6878 =====

^{*} The condition number is large (7e+03). This might indicate strong multicollinearity or other numerical problems.

3.6.5 Non-linear Transformations of the Predictors

The ols function can also accommodate non-linear transformations of the predictors. For example, given a predictor X, we can create predictor X^2 using I(X ** 2). We now perform a regression of medv onto lstat and lstat².

The near-zero p-value associated with the quadratic term suggests that it leads to an improve model. We use <code>anova_lm()</code> function to further quantify the extent to which the quadratic fit is superior to the linear fit. The null hypothesis is that the two models fit the data equally well. The alternative hypothesis is that the full model is superior. Given the large F-statistic and zero p-value, this provides very clear evidence that the model with quadratic term is superior. A plot of residuals versus fitted values shows that, with quadratic term included, there is no discernible pattern in residuals.

import statsmodels.formula.api as smf
from statsmodels import datasets
import statsmodels.api as sm
lowess = sm.nonparametric.lowess

```
import matplotlib.pyplot as plt
boston = datasets.get_rdataset('Boston', 'MASS').data
my_reg = smf.ols(formula='medv ~ lstat', data=boston)
my_fit = my_reg.fit()
my_reg2 = smf.ols(formula='medv ~ lstat + I(lstat ** 2)', data=boston)
my_fit2 = my_reg2.fit()
print(my_fit.summary2())
print('----')
print(sm.stats.anova_lm(my_fit2))
print('----')
print(sm.stats.anova_lm(my_fit, my_fit2))
my_regs = (my_reg, my_reg2)
fig = plt.figure(figsize=(8,4))
i_reg = 1
for reg in my_regs:
    ax = fig.add_subplot(1, 2, i_reg)
    fit = reg.fit()
    ax.scatter(fit.fittedvalues, fit.resid, s=7, alpha=0.6)
    lowess_fit = lowess(fit.resid, fit.fittedvalues)
    ax.plot(lowess_fit[:,0], lowess_fit[:,1], c='r')
    ax.axhline(y=0, linestyle='--', color='grey')
    ax.set_xlabel('Fitted values')
    ax.set_ylabel('Residuals')
    ax.set_title(reg.formula)
    i_reg += 1
fig.tight_layout()
                 Results: Ordinary least squares
Model:
                    OLS
                                     Adj. R-squared:
                                                         0.543
Dependent Variable: medv
                                     AIC:
                                                         3286.9750
Date:
                    2019-05-29 12:41 BIC:
                                                         3295.4280
```

No. Observati Df Model: Df Residuals: R-squared:	1 50 0.)4 . 544	F-st Prob Scal	tatistic: o (F-stat le:	istic): 5. 38	1.6 08e-88 .636
	Coef.	Std.Err.	t	P> t	[0.025	0.975]
Intercept lstat	34.5538 -0.9500	0.5626 0.0387	61.4151 -24.5279	0.0000	33.4485	35.6592 -0.8740
Omnibus: Prob(Omnibus) Skew: Kurtosis:	: (1 5	137.043 0.000 1.453 5.319	Durbin Jarque Prob(, Condit	n-Watson: e-Bera (J JB): tion No.:	TB):	0.892 291.373 0.000 30
	df	sum	_sq	mean_sq		F PR(>F)
						4 8.819026e-103
I(lstat ** 2)	1.0	4125.1382	260 4125	5.138260	135.19982	2 7.630116e-28
Residual	503.0	15347.243	158 30	0.511418	Na	N NaN
df_resid		ssr df_d:	iff ss	s_diff	F	Pr(>F)
0 504.0						
						7.630116e-28

3.6.6 Qualitative Predictors

We will now examine Carseats data, which is part of the ISLR library. We will attempt to predict Sales (child car seat sales) based on a number of predictors. statsmodels automatically converts string variables into categorical variables. If we want statsmodels to treat a numerical variable x as qualitative predictor, the formula should be y $^{\sim}$ C(x). Here C() stands for categorical.

```
import statsmodels.formula.api as smf
from statsmodels import datasets
```

carseats = datasets.get_rdataset('Carseats', 'ISLR').data
print(carseats.columns)

```
print('----')
all_columns = list(carseats.columns)
all_columns.remove('Sales')
my_formula = 'Sales ~ ' + ' + '.join(all_columns)
my_formula += ' + Income:Advertising + Price:Age'
print(my_formula)
print('----')
my_reg = smf.ols(formula=my_formula, data=carseats)
my_fit = my_reg.fit()
print(my_fit.summary2())
Index(['Sales', 'CompPrice', 'Income', 'Advertising', 'Population', 'Price',
      'ShelveLoc', 'Age', 'Education', 'Urban', 'US'],
     dtype='object')
_____
Sales ~ CompPrice + Income + Advertising + Population + Price + ShelveLoc +
Age + Education + Urban + US + Income: Advertising + Price: Age
-----
                Results: Ordinary least squares
Model:
                    OLS
                                   Adj. R-squared:
                                                     0.872
                                   AIC:
Dependent Variable: Sales
                                                     1157.3378
Date:
                   2019-05-29 12:53 BIC:
                                                     1213.2183
                                   Log-Likelihood:
No. Observations: 400
                                                     -564.67
Df Model:
                                   F-statistic:
                   13
                                                     210.0
Df Residuals:
                   386
                                   Prob (F-statistic): 6.14e-166
R-squared:
                    0.876
                                   Scale:
                                            1.0213
                   Coef. Std.Err. t  P>|t|  [0.025  0.975]
______
Intercept
                   6.5756 1.0087 6.5185 0.0000 4.5922 8.5589
ShelveLoc[T.Good] 4.8487 0.1528 31.7243 0.0000 4.5482 5.1492
ShelveLoc[T.Medium] 1.9533 0.1258 15.5307 0.0000 1.7060 2.2005
Urban[T.Yes]
                 0.1402  0.1124  1.2470  0.2132  -0.0808  0.3612
US[T.Yes]
                -0.1576   0.1489   -1.0580   0.2907   -0.4504   0.1352
CompPrice
                 0.0929  0.0041  22.5668  0.0000  0.0848  0.1010
Income
                   0.0109
                           0.0026 4.1828 0.0000 0.0058 0.0160
```

Advertising	0.0702	0.0226	3.1070	0.0020	0.0258	0.1147
Population	0.0002	0.0004	0.4329	0.6653	-0.0006	0.0009
Price	-0.1008	0.0074	-13.5494	0.0000	-0.1154	-0.0862
Age	-0.0579	0.0160	-3.6329	0.0003	-0.0893	-0.0266
Education	-0.0209	0.0196	-1.0632	0.2884	-0.0594	0.0177
Income:Advertising	0.0008	0.0003	2.6976	0.0073	0.0002	0.0013
Price:Age	0.0001	0.0001	0.8007	0.4238	-0.0002	0.0004
Omnibus:	1.281		Durbin-Wa	atson:		2.047
<pre>Prob(Omnibus):</pre>	0.527		Jarque-Be	era (JB)):	1.147
Skew:	0.129		Prob(JB)	:		0.564
Kurtosis:	3.050		Condition	n No.:		130576
=======================================	========	======		======		======

* The condition number is large (1e+05). This might indicate strong multicollinearity or other numerical problems.

3.6.7 Calling R from Python

4 Classification

4.1 An Overview of Classification

In figure 37, we have plotted annual income and monthly credit card balance for a subset of individuals in Credit data set. The left hand panel displays individuals who defaulted in brown, and those who did not in blue. We have plotted only a fraction of individuals who did not default. It appears that individuals who defaulted tended to have higher credit card balances than those who did not. In the right hand panel, we show two pairs of boxplots. The first shows the distribution of balance split by the binary default variable; the second is a similar plot for income.

4.2 Why Not Linear Regression?

4.3 Logistic Regression

Using Default data set, in figure 38 we show probability of default as a function of balance. The left panel shows a model fitted using linear regression. Some of the probabilities estimates (for low balance) are outside the [0, 1] interval. The right panel shows a model fitted using logistic regression, which models the probability of default as a function of balance. Now all probability estimates are in the [0, 1] interval.

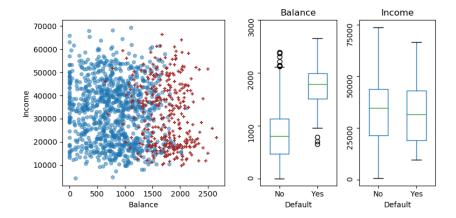


Figure 37: The Default data set. Left: The annual income and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card debt are shown in brown, and those who did not default are shown in blue. Center: Boxplots of balance as a function of default status. Right: Boxplots of income as a function of default status.

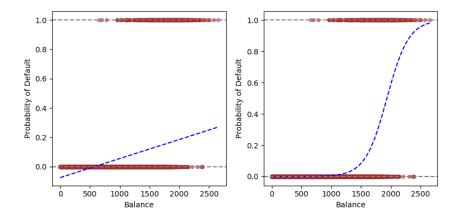


Figure 38: Classification using Default data. Left: Estimated probability of default using linear regression. Some estimated probabilities are negative! The brown ticks indicate the 0/1 values coded for default (No or Yes). Right: Predicted probabilities of default using logistic regression. All probabilities lie between 0 and 1.

Table 12 shows the coefficient estimates and related information that result from fitting a logistic regression model on the Default data in order to predict the probability of default = Yes using balance.

	Coef.	Std.Err.	z	$P > \mid z \mid$
Intercept	-10.6513	0.3612	-29.4913	0.0
balance	0.0055	0.0002	24.9524	0.0

Table 12: For the Default data, estimated coefficients of the logistic regression model that predicts the probability of default using balance. A one-unit increase in balance is associated with an increase in the log odds of default by 0.0055 units.

Table 13 shows the results of logistic model where default is a function of the qualitative variable student.

Table 14 shows the coefficient estimates for a logistic regression model that uses balance, income (in thousands of dollars), and student status to predict probability of default.

	Coef.	Std.Err.	z	$P > \mid z \mid$
Intercept	-3.5041	0.0707	-49.5541	0.0
student[T.Yes]	0.4049	0.115	3.5202	0.0004

Table 13: For the Default data, estimated coefficients of the logistic regression model that predicts the probability of default using student status.

	Coef.	Std.Err.	z	$P > \mid z \mid$
Intercept	-10.869	0.4923	-22.0793	0.0
student[T.Yes]	-0.6468	0.2363	-2.7376	0.0062
balance	0.0057	0.0002	24.7365	0.0
income	0.003	0.0082	0.3698	0.7115

Table 14: For the Default data, estimated coefficients of the logistic regression model that predicts the probability of default using balance, income, and student status. In fitting this model, income was measured in thousands of dollars.

The left hand panel of figure 39 shows average default rates for students and non-students, respectively, as a function of credit card balance. For a fixed value of balance and income, a student is less likely to default than a non-student. This is true for all values of balance. This is consistent

with negative coefficient of student in table 14. But the horizontal lines near the base of the plot, which show the default rates for students and non-students averaged over all values of balance and income, suggest the opposite effect: the overall student default rate is higher than non-student default rate. Consequently, there is a positive coefficient for student in the single variable logistic regression output shown in table 13.

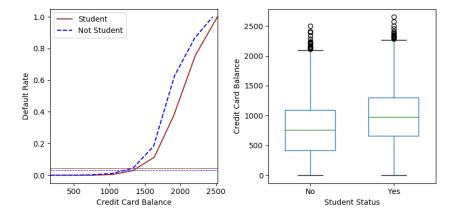


Figure 39: Confounding in the Default data. Left: Default rates are shown for students (brown) and non-students (blue). The solid lines display default rate as a function of balance, while the horizontal lines display the overall default rates. Right: Boxplots of balance for students and non-students are shown.

4.4 Linear Discriminant Analysis

In the left panel of figure 40, two normal density functions that are displayed, $f_1(x)$ and $f_2(x)$, represent two distinct classes. The Bayes classifier boundary, shown as vertical dashed line, is estimated using the function GaussianNB(). The right hand panel displays a histogram of a random sample of 20 observations from each class. The LDA decision boundary is shown as firm vertical line.

Two examples of multivariate Gaussian distributions with p=2 are shown in figure 41. In the upper panel, the height of the surface at any particular point represents the probability that both X_1 and X_2 fall in the small region around that point. If the surface is cut along the X_1 axis or along the X_2 axis, the resulting cross-section will have the shape of a one-dimensional normal distribution. The left-hand panel illustrates an example in which

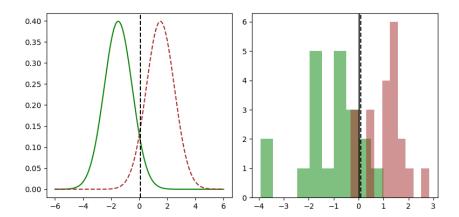


Figure 40: Left: Two one-dimensional normal density functions are shown. The dashed vertical line represents the Bayes decision boundary. Right: 20 observations were drawn from each of the two classes, and are shown as histograms. The Bayes decision boundary is again shown as a dashed vertical line. The solid vertical line represents the LDA decision boundary estimated from the training data.

 $var(X_1) = var(X_2)$ and $cor(X_1, X_2) = 0$; this surface has a characteristic bell shape. However, the bell shape will be distorted if the predictors are correlated or have unequal variances, as is illustrated in the right-hand panel of figure 41. In this situation, the base of the bell will have an elliptical, rather than circular, shape. The contour plots in the lower panel are not in the book.

Figure 42 shows an example of three equally sized Gaussian classes with class-specific mean vectors and a common covariance matrix. The dashed lines are the Bayes decision boundaries.

A confusion matrix, shown for the Default data in table 15, is a convenient way to display prediction of default in comparison to true default. Table 16 shows the error rates that result when we label any customer with a posterior probability of default above 20% to the default class.

Figure 43 illustrates the trade-off that results from modifying the threshold value for the posterior probability of default. Various error rates are shown as a function of the threshold value. Using a threshold of 0.5 minimizes the overall error rate, shown as a black line. But when a threshold of 0.5 is used, the error rate among the individuals who default is quite high (blue dashed line). As the threshold is reduced, the error rate among indi-

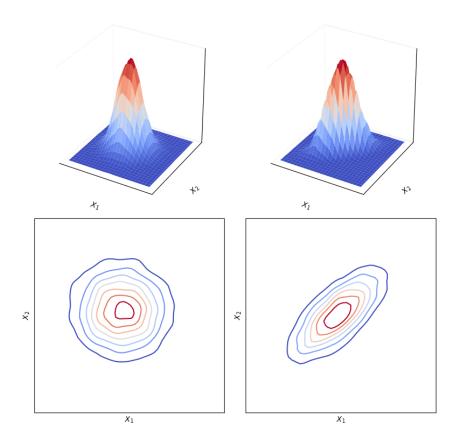


Figure 41: Two multivariate Gaussian density functions are shown, with p=2. Left: The two predictors are uncorrelated. Right: The two predictors have a correlation of 0.7. The lower panel shows contour plots of the surfaces drawn in the upper panel. Here the correlations can be easily seen.

	true No	true Yes	Total
predict No	9645	254	9899
predict Yes	22	79	101
Total	9667	333	10000

Table 15: A confusion matrix compares the LDA predictions to the true default statuses for the training observations in the Default data set. Elements of the diagonal matrix represent individuals whose default statuses were correctly predicted, while off-diagonal elements represent individuals that were missclassified.

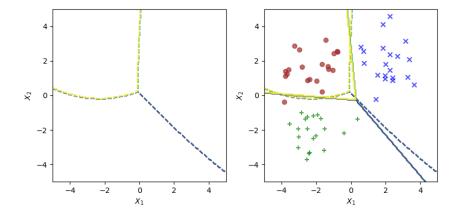


Figure 42: An example with three classes. The observation from each class are drawn from a multivariate Gaussian distribution with p=2, with a class-specific mean vector and a common covariance matrix. Left: The dashed lines are the Bayes decision boundaries. Right: 20 observations were generated from each class, and the corresponding LDA decision boundaries are indicated using solid black lines. The Bayes decision boundaries are once again shown as dashed lines.

	true No	true Yes	Total
predict No	9435	140	9575
predict Yes	232	193	425
Total	9667	333	10000

Table 16: A confusion matrix compares LDA predictions to the true default statuses for the training observations in the Default data set, using a modified threshold value that predicts default for any individuals whose posterior default probability exceeds 20%.

viduals who default decreases steadily, but the error rate amond individuals who do not default increases.

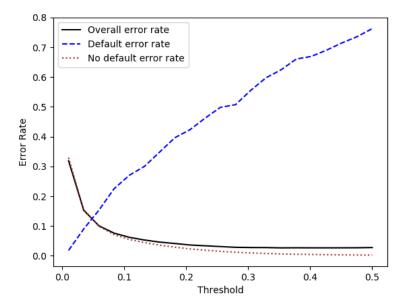


Figure 43: For the Default data set, error rates are shown as a function of the threshold value for the posterior probability that is used to perform the assignment of default. The black sold line displays the overall error rate. The blue dashed line represents the fraction of defaulting customers that are incorrectly classified, and the orange dotted line indicates the fraction of errors among the non-defaulting customers.

Figure 44 displays the ROC curve for the LDA classifier on the Default data set.

Table 17 shows the possible results when applying a classifier (or diagnostic test) to a population.

Table 18 lists many of the popular performance measures that are used in this context.

Figure 45 illustrates the performances of LDA and QDA in two scenarios. In the left-hand panel, the two Gaussian classes have a common correlation of 0.7 between X_1 and X_2 . As a result, the Bayes decision boundary is nearly linear and is accurately approximated by the LDA decision boundary. In contrast, the right-hand panel displays a situation in which the orange class

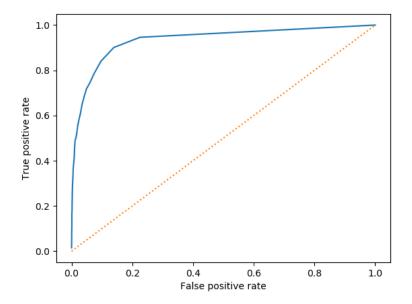


Figure 44: A ROC curve for the LDA classifier on the Default data. It traces two types of error as we vary the threshold value for the posterior probability of default. The actual thresholds are not shown. The true positive rate is the sensitivity: the fraction of defaulters that are correctly identified using a given threshold value. The false positive rate is the fraction of non-defaulters we incorrectly specify as defaulters, using the same threshold value. The ideal ROC curve hugs the top left corner, indicating a high true positive rate and a low false positive rate. The dotted line represents the "no information" classifier; this is what we would expect if student status and credit card balance are not associated with the probability of default.

		True class		
		- or Null	+ or Non-null	Total
Predicted	- or Null	True Negative (TN)	False Negative (FN)	N*
class	+ or Non-null	False Positive (FP)	True Positive (TP)	P*
	Total	N	Р	

Table 17: Possible results when applying a classifier or diagnostic test to a population.

Name	Definition	Synonyms
False Positive rate	FP / N	Type I error, 1 - specificity
True Positive rate	$\mathrm{TP} \ / \ \mathrm{P}$	1 - Type II error, power, sensitivity, recall
Positive Predicted value	TP / P^*	Precision, 1 - false discovery proportion
Negative Predicted value	TN / N*	

Table 18: Important measures for classification and diagnostic testing, derived from quantities in table 17.

has a correlation of 0.7 between the variables and blue class has a correlation of -0.7.

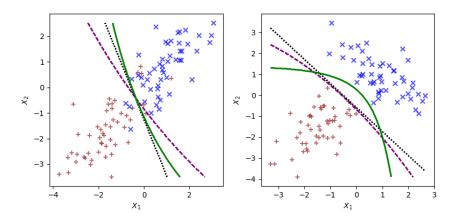


Figure 45: Left: The Bayes (purple dashed), LDA (black dotted), and QDA (green sold) decision boundaries for a two-class problem with $\Sigma_1 = \Sigma_2$. Right: Details are as given in the left-hand panel, except that $\Sigma_1 \neq \Sigma_2$.

4.5 A Comparison of Classification Methods

Figure 46 illustrates the performances of the four classification approaches (KNN, LDA, Logistic, and QDA) when Bayes decision boundary is linear.

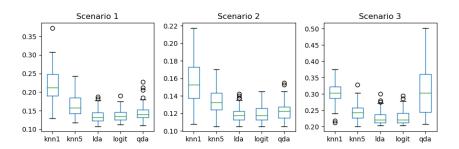


Figure 46: Boxplots of the test error rates for each of the linear scenarios described in the main text.

4.6 Lab: Logistic Regression, LDA, QDA, and KNN

4.6.1 The Stock Market Data

We will begin by examining some numerical and graphical summaries of the Smarket data, which is part of the ISLR library.

```
from statsmodels import datasets
import pandas as pd
smarket = datasets.get_rdataset('Smarket', 'ISLR').data
print(smarket.columns)
print('----')
print(smarket.shape)
print('----')
print(smarket.describe())
print('----')
print(smarket.iloc[:,1:8].corr())
print('----')
smarket.boxplot(column='Volume', by='Year', grid=False)
Index(['Year', 'Lag1', 'Lag2', 'Lag3', 'Lag4', 'Lag5', 'Volume', 'Today',
       'Direction'],
     dtype='object')
(1250, 9)
_____
             Year
                          Lag1
                                          Volume
                                                        Today
```

```
1250.000000
                    1250.000000
                                       1250.000000 1250.000000
count
mean
       2003.016000
                       0.003834
                                  . . .
                                          1.478305
                                                        0.003138
std
          1.409018
                       1.136299
                                          0.360357
                                                        1.136334
min
       2001.000000
                      -4.922000
                                          0.356070
                                                       -4.922000
                                  . . .
25%
       2002.000000
                      -0.639500
                                          1.257400
                                                       -0.639500
50%
       2003.000000
                       0.039000
                                          1.422950
                                                       0.038500
                                  . . .
75%
       2004.000000
                       0.596750
                                          1.641675
                                                       0.596750
       2005.000000
                       5.733000
                                          3.152470
                                                       5.733000
max
                                 . . .
```

[8 rows x 8 columns]

	Lag1	Lag2	Lag3	Lag4	Lag5	Volume	Today	
Lag1	1.000000	-0.026294	-0.010803	-0.002986	-0.005675	0.040910	-0.026155	
Lag2	-0.026294	1.000000	-0.025897	-0.010854	-0.003558	-0.043383	-0.010250	
Lag3	-0.010803	-0.025897	1.000000	-0.024051	-0.018808	-0.041824	-0.002448	
Lag4	-0.002986	-0.010854	-0.024051	1.000000	-0.027084	-0.048414	-0.006900	
Lag5	-0.005675	-0.003558	-0.018808	-0.027084	1.000000	-0.022002	-0.034860	
Volume	0.040910	-0.043383	-0.041824	-0.048414	-0.022002	1.000000	0.014592	
Today	-0.026155	-0.010250	-0.002448	-0.006900	-0.034860	0.014592	1.000000	

4.6.2 Logistc Regression

Next, we will fit a logistic regression model to predict Direction using Lag1 through Lag5 and Volume.

```
from statsmodels import datasets
import statsmodels.formula.api as smf
import numpy as np
import pandas as pd

smarket = datasets.get_rdataset('Smarket', 'ISLR').data
smarket['direction_cat'] = smarket['Direction'].apply(lambda x: int(x=='Up'))

logit_model = smf.logit(
    formula='direction_cat ~ Lag1 + Lag2 + Lag3 + Lag4 + Lag5 + Volume',
    data=smarket)

logit_fit = logit_model.fit()

print(logit_fit.summary2())
```

```
print('----')
print(dir(logit_fit))
                 # see what information is available from fit
print('----')
print(logit_fit.params)
                      # coefficients estimates
print('----')
print(logit_fit.summary2().tables[1]) # coefficients estimates, std error, and z
print('----')
print(logit_fit.summary2().tables[1].iloc[:,3]) # P > |z| column only
print('----')
print(logit_fit.predict()[:10]) # probabilities for training data
print('----')
smarket['predict_direction'] = np.vectorize(
   lambda x: 'Up' if x > 0.5 else 'Down')(logit_fit.predict())
print(pd.crosstab(smarket['predict_direction'], smarket['Direction']))
Optimization terminated successfully.
      Current function value: 0.691034
      Iterations 4
                  Results: Logit
______
Model:
                          Pseudo R-squared: 0.002
              Logit
Dependent Variable: direction_cat
                          AIC:
                                        1741.5841
              2019-06-06 18:56 BIC:
                                       1777.5004
No. Observations: 1250
                          Log-Likelihood: -863.79
Df Model:
                          LL-Null:
                                       -865.59
Df Residuals:
             1243
                                      0.73187
                          LLR p-value:
Converged:
             1.0000
                          Scale:
                                        1.0000
No. Iterations: 4.0000
          Coef. Std.Err. z P>|z| [0.025 0.975]
_____
                  0.2407 -0.5234 0.6007 -0.5978 0.3458
Intercept
         -0.1260
         -0.0731 0.0502 -1.4566 0.1452 -0.1714 0.0253
Lag1
Lag2
         Lag3
         0.0111 0.0499 0.2220 0.8243 -0.0868 0.1090
         Lag4
Lag5
          Volume
```

```
_____
['__class__', '__delattr__', '__dict__', '__dir__', '__doc__', '__eq__',
'__format__', '__ge__', '__getattribute__', '__getstate__', '__gt__',
'_hash__', '__init__', '__init_subclass__', '__le__', '__lt__',
'__module__', '__ne__', '__new__', '__reduce__', '__reduce_ex__', '__repr__',
'__setattr__', '__sizeof__', '__str__', '__subclasshook__', '__weakref__',
'_cache', '_data_attr', '_get_endog_name', '_get_robustcov_results', 'aic',
'bic', 'bse', 'conf_int', 'cov_kwds', 'cov_params', 'cov_type', 'df_model',
'df_resid', 'f_test', 'fittedvalues', 'get_margeff', 'initialize',
'k_constant', 'llf', 'llnull', 'llr', 'llr_pvalue', 'load', 'mle_retvals',
'mle_settings', 'model', 'nobs', 'normalized_cov_params', 'params',
'pred_table', 'predict', 'prsquared', 'pvalues', 'remove_data', 'resid_dev',
'resid_generalized', 'resid_pearson', 'resid_response', 'save', 'scale',
'set_null_options', 'summary', 'summary2', 't_test', 't_test_pairwise',
'tvalues', 'use_t', 'wald_test', 'wald_test_terms']
-----
Intercept
           -0.126000
Lag1
           -0.073074
Lag2
           -0.042301
Lag3
            0.011085
Lag4
            0.009359
Lag5
            0.010313
Volume
            0.135441
dtype: float64
-----
             Coef.
                    Std.Err.
                                          P>|z|
                                                   [0.025
                                                             0.975]
                                    Z
Intercept -0.126000
                    0.240737 - 0.523394 \quad 0.600700 - 0.597836 \quad 0.345836
Lag1
         -0.073074
                    0.050168 - 1.456583 \quad 0.145232 - 0.171401 \quad 0.025254
         -0.042301
Lag2
                    0.050086 - 0.844568 \quad 0.398352 - 0.140469 \quad 0.055866
Lag3
          0.011085
                    0.049939 0.221974 0.824334 -0.086793 0.108963
Lag4
                    0.009359
Lag5
          0.010313
                    Volume
          0.135441 0.158361 0.855266 0.392404 -0.174941 0.445822
-----
Intercept
            0.600700
Lag1
            0.145232
Lag2
            0.398352
Lag3
            0.824334
Lag4
            0.851445
Lag5
            0.834998
```

```
0.392404
Volume
Name: P>|z|, dtype: float64
[0.50708413 0.48146788 0.48113883 0.51522236 0.51078116 0.50695646
 0.49265087 0.50922916 0.51761353 0.48883778]
Direction
                   Down
                          Uр
predict_direction
Down
                    145 141
                    457 507
Uр
   We now use data for years 2001 through 2004 to train the model, then
use data for year 2005 to test the model.
from statsmodels import datasets
import statsmodels.formula.api as smf
import pandas as pd
import numpy as np
smarket = datasets.get_rdataset('Smarket', 'ISLR').data
smarket['direction_cat'] = smarket['Direction'].apply(lambda x:
      int(x == 'Up'))
smarket_train = smarket.loc[smarket['Year'] < 2005]</pre>
smarket_test = smarket.loc[smarket['Year'] == 2005].copy()
logit_model = smf.logit(
    formula='direction_cat ~ Lag1 + Lag2 + Lag3 + Lag4 + Lag5 + Volume',
    data=smarket_train)
logit_fit = logit_model.fit()
prob_up_test = logit_fit.predict(smarket_test)
smarket_test.loc[:,'direction_predict'] = np.vectorize(
    lambda x: 'Up' if x > 0.5 else 'Down')(prob_up_test)
confusion_test = \
    pd.crosstab(smarket_test['direction_predict'], smarket_test['Direction'])
print(confusion_test)
print('----')
print(np.mean(np.mean(smarket_test['direction_predict'] ==
      smarket_test['Direction'])))
```

```
print('----')
# Refit logistic regression with only Lag1 and Lag2
logit_model = smf.logit('direction_cat ~ Lag1 + Lag2', data=smarket_train)
logit_fit = logit_model.fit()
prob_up_test = logit_fit.predict(smarket_test)
smarket_test['direction_pred_2var'] = np.vectorize(
   lambda x: 'Up' if x > 0.5 else 'Down')(prob_up_test)
print(pd.crosstab(smarket_test['direction_pred_2var'],
  smarket_test['Direction']))
print('----')
print(np.mean(smarket_test['direction_pred_2var'] == smarket_test['Direction']))
print('----')
print(logit_fit.predict(exog=dict(Lag1=[1.2,1.5], Lag2=[1.1,-0.8])))
Optimization terminated successfully.
         Current function value: 0.691936
         Iterations 4
Direction
                  Down Up
direction_predict
Down
                    77 97
Uр
                    34 44
_____
0.4801587301587302
_____
Optimization terminated successfully.
         Current function value: 0.692085
         Iterations 3
Direction
                    Down
                           Uр
direction_pred_2var
Down
                      35
                            35
Uр
                      76 106
-----
0.5595238095238095
    0.479146
    0.496094
```

dtype: float64

4.6.3 Linear Discriminant Analysis

Now we will perform LDA on Smarket data.

```
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA
from statsmodels import datasets
import pandas as pd
import numpy as np
smarket = datasets.get_rdataset('Smarket', 'ISLR').data
smarket_train = smarket.loc[smarket['Year'] < 2005]</pre>
smarket_test = smarket.loc[smarket['Year'] == 2005].copy()
lda_model = LDA()
lda_fit = lda_model.fit(smarket_train[['Lag1', 'Lag2']],
smarket_train['Direction'])
print(lda_fit.priors_)
                               # Prior probabilities of groups
print('----')
print(lda_fit.means_)
                               # Group means
print('----')
print(lda_fit.scalings_)
                               # Coefficients of linear discriminants
print('----')
lda_predict_2005 = lda_fit.predict(smarket_test[['Lag1', 'Lag2']])
print(pd.crosstab(lda_predict_2005, smarket_test['Direction']))
print('----')
print(np.mean(lda_predict_2005 == smarket_test['Direction']))
print('----')
lda_predict_prob2005 = lda_fit.predict_proba(smarket_test[['Lag1', 'Lag2']])
print(np.sum(lda_predict_prob2005[:,0] >= 0.5))
print(np.sum(lda_predict_prob2005[:,0] < 0.5))</pre>
[0.49198397 0.50801603]
-----
[[ 0.04279022  0.03389409]
 [-0.03954635 -0.03132544]]
-----
[[-0.64201904]
 [-0.51352928]]
```

```
-----
Direction Down
                  Uр
row_0
Down
             35
                  35
             76 106
Uр
0.5595238095238095
-----
70
182
4.6.4 Quadratic Discriminant Analysis
We will now fit a QDA model to the Smarket data.
from statsmodels import datasets
from \ sklearn. discriminant\_analysis \ import \ Quadratic Discriminant Analysis \ as \ QDA
import pandas as pd
import numpy as np
smarket = datasets.get_rdataset('Smarket', 'ISLR').data
smarket_train = smarket.loc[smarket['Year'] < 2005]</pre>
smarket_test = smarket.loc[smarket['Year'] == 2005].copy()
qdf = QDA()
qdf.fit(smarket_train[['Lag1', 'Lag2']], smarket_train['Direction'])
                                # Prior probabilities of groups
print(qdf.priors_)
print('----')
print(qdf.means_)
                                # Group means
print('----')
predict_direction2005 = qdf.predict(smarket_test[['Lag1', 'Lag2']])
print(pd.crosstab(predict_direction2005, smarket_test['Direction']))
print('----')
print(np.mean(predict_direction2005 == smarket_test['Direction']))
[0.49198397 0.50801603]
-----
[[ 0.04279022  0.03389409]
 [-0.03954635 -0.03132544]]
```

```
Direction Down Up
row_0
Down 30 20
Up 81 121
------0.5992063492063492
```

4.6.5 K-Nearest Neightbors

We will now perform KNN, also on the Smarket data.

```
from statsmodels import datasets
from sklearn.neighbors import KNeighborsClassifier
import pandas as pd
import numpy as np
smarket = datasets.get_rdataset('Smarket', 'ISLR').data
smarket_train = smarket.loc[smarket['Year'] < 2005]</pre>
smarket_test = smarket.loc[smarket['Year'] == 2005].copy()
knn1 = KNeighborsClassifier(n_neighbors=1)
knn1.fit(smarket_train[['Lag1', 'Lag2']], smarket_train['Direction'])
smarket_test['predict_dir_knn1'] = knn1.predict(smarket_test[['Lag1', 'Lag2']])
print(pd.crosstab(smarket_test['predict_dir_knn1'], smarket_test['Direction']))
print('----')
print(np.mean(smarket_test['predict_dir_knn1'] == smarket_test['Direction']))
print('----')
knn3 = KNeighborsClassifier(n_neighbors=3)
knn3.fit(smarket_train[['Lag1', 'Lag2']], smarket_train['Direction'])
smarket_test['predict_dir_knn3'] = knn3.predict(smarket_test[['Lag1', 'Lag2']])
print(pd.crosstab(smarket_test['predict_dir_knn3'], smarket_test['Direction']))
print('----')
print(np.mean(smarket_test['predict_dir_knn3'] == smarket_test['Direction']))
Direction
                  Down Up
predict_dir_knn1
Down
                    43 58
Uр
                    68 83
_____
0.5
```

```
Direction Down Up predict_dir_knn3

Down 48 55

Up 63 86
-----
0.5317460317460317
```

4.6.6 An Application to Caravan Insurance Data

Finally, we will apply the KNN approach to the Caravan data set in the ISLR library.

```
from statsmodels import datasets
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import LogisticRegression
import pandas as pd
import numpy as np
caravan = datasets.get_rdataset('Caravan', 'ISLR').data
print(caravan['Purchase'].value_counts())
print('----')
caravan_scale = caravan.iloc[:,:-1]
caravan_scale = (caravan_scale - caravan_scale.mean()) / caravan_scale.std()
caravan_test = caravan_scale.iloc[:1000]
purchase_test = caravan.iloc[:1000]['Purchase']
caravan_train = caravan_scale.iloc[1000:]
purchase_train = caravan.iloc[1000:]['Purchase']
# Fit KNN with 1, 3, and 5 neighbors
knn1 = KNeighborsClassifier(n_neighbors=1)
knn1.fit(caravan_train, purchase_train)
purchase_predict_knn1 = knn1.predict(caravan_test)
print(np.mean(purchase_test != purchase_predict_knn1))
print('----')
print(np.mean(purchase_test == 'Yes'))
```

```
print('----')
print(pd.crosstab(purchase_predict_knn1, purchase_test))
print('----')
knn3 = KNeighborsClassifier(n_neighbors=3)
knn3.fit(caravan_train, purchase_train)
purchase_predict_knn3 = knn3.predict(caravan_test)
print(np.mean(purchase_test != purchase_predict_knn3))
print('----')
print(np.mean(purchase_test == 'Yes'))
print('----')
print(pd.crosstab(purchase_predict_knn3, purchase_test))
print('----')
knn5 = KNeighborsClassifier(n_neighbors=5)
knn5.fit(caravan_train, purchase_train)
purchase_predict_knn5 = knn5.predict(caravan_test)
print(np.mean(purchase_test != purchase_predict_knn5))
print('----')
print(np.mean(purchase_test == 'Yes'))
print('----')
print(pd.crosstab(purchase_predict_knn5, purchase_test))
print('----')
# Now fit logistic regression
logit_model = LogisticRegression(solver='lbfgs', max_iter=1000)
logit_model.fit(caravan_train, purchase_train)
purchase_predict_logit = logit_model.predict(caravan_test)
print(pd.crosstab(purchase_predict_logit, purchase_test))
print('----')
purchase_predict_prob_logit = logit_model.predict_proba(caravan_test)
purchase_predict_logit_prob25 = np.vectorize(
    lambda x: 'Yes' if x > 0.25 else 'No')(purchase_predict_prob_logit[:,1])
print(pd.crosstab(purchase_predict_logit_prob25, purchase_test))
No
      5474
Yes
       348
```

```
Name: Purchase, dtype: int64
_____
0.118
_____
0.059
_____
Purchase
          No Yes
row_0
         873
No
               50
Yes
          68
                9
0.074
-----
0.059
-----
Purchase
          No Yes
row_0
No
         921
               54
          20
Yes
                5
-----
0.066
-----
0.059
-----
Purchase
          No
             Yes
row_0
No
         930
               55
Yes
          11
                4
_____
Purchase
          No
              Yes
row_0
         934
               59
No
                0
Yes
Purchase
          No Yes
row_0
No
         917
               48
          24
Yes
               11
```

5 Resampling Methods

5.1 Cross-Validation

Figure 47 displays the *validation set approach*, a simple stategy to estimate the test error associated with fitting a particular statistical learning method on a set of observations.

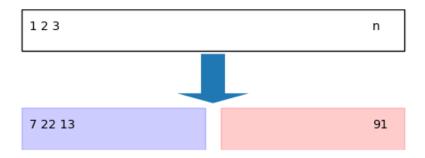


Figure 47: A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in red, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.

In figure 48, the left-hand panel shows validation sample MSE as a function of polynomial order for which a regression model was fit on training sample. The two samples are obtained by randomly splitting Auto data set into two data sets of 196 observations each. The right-hand panel shows the results of repeating this exercise 10 times, each time with a different random split of the observations into training and validation sets. The model with a quadratic term has a lower MSE compared to the model with only a linear term. There is not much benefit from adding cubic or higher order polynomial terms in the regression model.

Figure 49 displas the Leave One Out Cross Validation (LOOCV) approach.

The left-hand panel of figure 50 shows test set MSE as a function of polynomial degree when LOOCV is used on the Auto data set. We fit linear regression models to predict mpg using polynomial functions of horsepower. The right-hand panel of figure 50 shows nine different 10-fold CV estimates

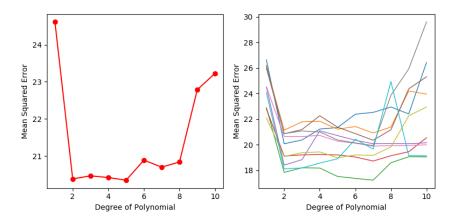


Figure 48: The validation set approach was used in the Auto data set in order to estimate the test error that results from predicting mpg using polynomial functions of horsepower. Left: Validation error estimates for a single split into training and validation data sets. Right: The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability of of the estimated test MSE that results from this approach.

for the Auto data set, each resulting from a different random split of the observations into ten folds.

Figure 51 illustrates the k-fold CV approach.

In figure 52, we plot the cross-validation estimates and true test error rates that result from fitting least squares polynomials to the simulated data sets illustrated in figures 9, 10, and 11 of chapter 2. In all three plots, the two cross validation errors are very similar.

Figure 53 shows Bayesian decision boundary (blue dashed line) and logistic regression decision boundary (black line) for 1- to 4-degree polynomials on X_1 and X_2 .

The left-hand panel of figure 54 displays in black 10-fold CV error rates that result from fitting ten logistic regression models to the data, using polynomial functions of the predictors up to tenth order. The true test errors are shown in red, and the training errors are shown in blue. The training error tends to decrease as the flexibility of the fit increases. The test error is higher than training error. The 10-fold CV error rate is a close approximation to the test error rate.

The right-hand panel of figure 54 displays the same three curves using

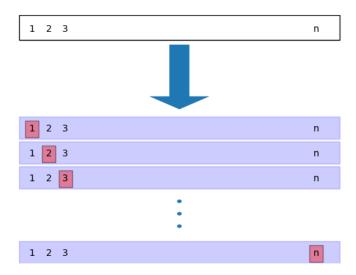


Figure 49: A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in red). The test error is then estimated by averaging the n resulting MSE's. The first training set contains all but observation 1, the second training set contains all but observation 2, and so on.

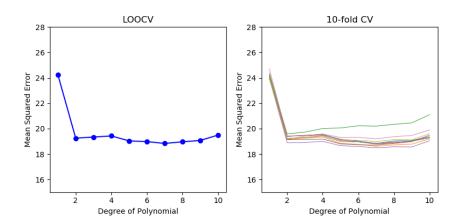


Figure 50: Cross-validation was used in the Auto data set in order to estimate the test error that results from predicting mpg using polynomial functions of horsepower. Left: The LOOCV error curve. Right: 10-fold CV was run nin separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.

the KNN approach for classification, as a function of the value of K (the number of neighbors used in the KNN classifier). Again, the training error rate declines as the method becomes more flexible, and so we see that the training error rate cannot be used to select the optimal value of K.

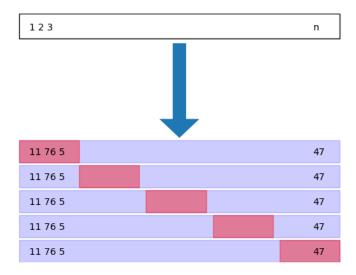


Figure 51: A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in red), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.

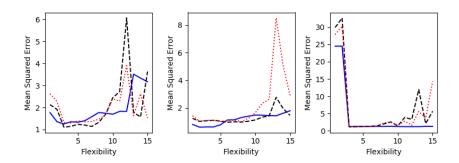


Figure 52: True and estimated test MSE for the simulated data sets in Figures 9 (left), 10 (center), and 11 (right). The true test MSE is shown in blue, the LOOCV estimate is shown in black dashed line, and the 10-fold CV estimate is shown in red dotted line.

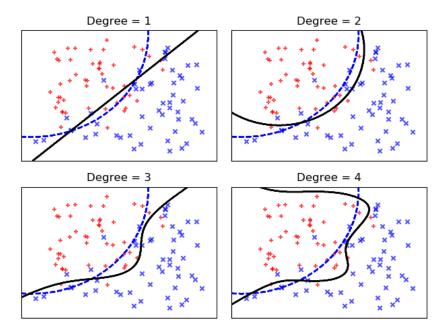


Figure 53: Logistic regression fits on the two-dimensional classification data displayed in figure 13. The Bayes decision boundary is represented using a blue dashed line. Estimated decision boundaries from linear, quadratic, cubic, and quartic (degrees 1-4) logistic regressions are displayed in black.

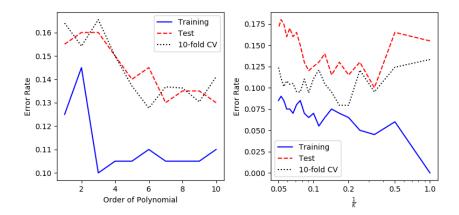


Figure 54: Test error (red), training error(blue), and 10-fold CV error (black) on the two-dimensional classification data displayed in 53. Left: Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x-axis. Right: The KNN classifier with different values of K, the number of neighbors used in the KNN classifier.

5.2 The Bootstrap

Figure 55 illustrates the approach for estimating α by repeated simulation of data. In each panel, we simulated 100 pairs of returns for the investments X and Y. We used these returns to estimate σ_X^2 , σ_Y^2 and σ_{XY} , which are then used to estimate α .

It is natural to wish to quantify the accuracy of our estimate of α . To estimate the standard deviation of $\hat{\alpha}$, we repeated the process of simulating 100 paired observations of X and Y, and estimating α 1000 times. We thereby obtain 1000 estimates of α , which we can call $\hat{\alpha}_1, \hat{\alpha}_2, ..., \hat{\alpha}_{1000}$. The left-hand panel of figure 56 displays a histogram of the resulting estimates. The mean over all 1000 estimates for α is 0.599, which is very close to $\alpha = 0.6$. The standard deviation of the estimates is 0.08.

The bootstrap approach is illustrated in the center panel of figure 56, which displays a histogram of 1000 bootstrap estimates of α , each computed using a distinct bootstrap data set. The panel was constructed on the basis of a single data set, and hence could be created using real data. The right-hand panel displays the information in the center and left panels in a different way, via boxplots of the estimates of α obtained by generating 1000 simulated data sets from the true population and using the boostrap approach.

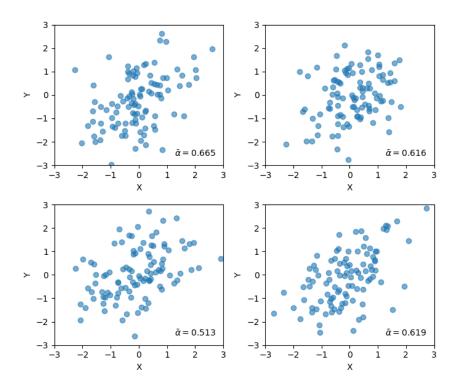


Figure 55: Each panel displays 100 simulated returns for investments X and Y. The resulting estimates of α are displayed in bottom right corner.

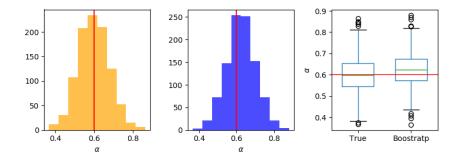


Figure 56: Left: A histogram of the estimates of α obtained by generating 1000 simulated data sets from the true population. Center: A histogram of the estimates of α obtained from 1000 bootstrap samples from a single data set. Right: The estimates of α displayed in the left and center panels are shown as boxplots. In each panel, the red line indicates the true value of α .

5.3 Lab: Cross-Validation and the Bootstrap

5.3.1 The Validation Set Approach

We use the function **choice** in numpy.random library to split the set of observations in Auto data set into two subsets of 196 observations. Then we fit regression models on the training data set and calculate validation error on the validation set.

These results show that a model that predicts mpg using a quadratic function of horsepower performs better than a model that predicts mpg using a linear function of horsepower. There is little evidence that a cubic function of horsepower is better than the quadratic function.

```
import numpy as np
from statsmodels import datasets
import statsmodels.formula.api as smf
auto = datasets.get_rdataset('Auto', 'ISLR').data
np.random.seed(911)
train_ind = np.random.choice(auto.shape[0], size=int(auto.shape[0]/2),
     replace=False)
all_ind = np.arange(auto.shape[0])
test_ind = set(all_ind).difference(set(train_ind))
test_ind = list(test_ind)
auto_train = auto.iloc[train_ind]
auto_test = auto.iloc[test_ind]
# Fit first linear model
lm_model = smf.ols(formula='mpg ~ horsepower', data=auto_train)
lm_fit = lm_model.fit()
mse_train = np.sum((lm_fit.predict(auto_train) - auto_train['mpg']) ** 2) / \
    (auto_train.shape[0] - 2)
print(mse_train)
print(lm_fit.mse_resid)
                                # same value
print('----')
mse_test = np.sum((lm_fit.predict(auto_test) - auto_test['mpg']) ** 2) / \
    (auto_test.shape[0] - 2)
print(mse_test)
print('----')
```

```
# Fit quadratic model
lm_model2 = smf.ols('mpg ~ horsepower + I(horsepower ** 2)', data=auto_train)
lm_fit2 = lm_model2.fit()
mse_test2 = np.sum((lm_fit2.predict(auto_test) - auto_test['mpg']) ** 2) / \
    (auto_test.shape[0] - 3)
print(mse_test2)
print('----')
# Fit third order polynomial model
lm_model3 = smf.ols('mpg ~ horsepower + I(horsepower ** 2) + I(horsepower ** 3)',
    data=auto_train)
lm_fit3 = lm_model3.fit()
mse_test3 = np.sum((lm_fit3.predict(auto_test) - auto_test['mpg']) ** 2) / \
    (auto_test.shape[0] - 4)
print(mse_test3)
23.61593457249045
23.615934572490445
_____
24.868027221207488
-----
20.701029881139203
20.893010200297326
```

5.3.2 Leave-One-Out Cross-Validation

mseLOOCV.py

Using first principles, it is straightforward to implement leave-one-out cross-validation.

```
import numpy as np
from statsmodels import datasets
import statsmodels.formula.api as smf

auto = datasets.get_rdataset('Auto', 'ISLR').data
all_ind = np.arange(auto.shape[0])

my_formula = 'mpg ~ horsepower'
```

```
mse_loocv = []
degree = []
for i_degree in range(1, 6):
    mse = []
    for i_obs in range(auto.shape[0]):
# auto_train = auto.loc[all_ind != i_obs]
auto_train = auto.drop(auto.index[i_obs])
auto_test = auto.iloc[i_obs]
lm_model = smf.ols(my_formula, data=auto_train)
lm_fit = lm_model.fit()
hp_predict = lm_fit.predict(
    exog=dict(horsepower=auto_test['horsepower']))
mse.append((hp_predict - auto_test['mpg']) ** 2)
    mse_loocv.append(np.mean(mse))
    degree.append(i_degree)
    my_formula += ' + I(horsepower **' + str(i_degree + 1) + ')'
for i_degree, mse in zip(degree, mse_loocv):
    print('degree: ', i_degree, ', mse_loocv:', round(mse, 3))
import sys
sys.path.append('code/chap5/')
import mseLOOCV
degree: 1 , mse_loocv: 24.232
degree: 2 , mse_loocv: 19.248
degree: 3 , mse_loocv: 19.335
degree: 4 , mse_loocv: 19.424
degree: 5 , mse_loocv: 19.033
```

5.3.3 k-Fold Cross-Validation

Using first principles, it is straightforward to implement k-fold CV. Once again, we see little evidence that using cubic or higher order polynomial terms leads to lower test error than simply using a quadratic fit.

```
# mse_kFoldCV.py
```

```
import numpy as np
import statsmodels.formula.api as smf
from statsmodels import datasets
auto = datasets.get_rdataset('Auto', 'ISLR').data
n_folds = 10
max_degree = 10
np.random.seed(911)
fold_ind = np.random.choice(n_folds, auto.shape[0])
all_ind = np.arange(auto.shape[0])
degree = []
mse_folds = {}
my_formula = 'mpg ~ horsepower'
for i_degree in range(1, max_degree + 1):
    mse_folds[i_degree] = []
    for i_fold in range(n_folds):
train_df = auto.loc[i_fold != fold_ind]
test_df = auto.loc[i_fold == fold_ind]
lm_model = smf.ols(my_formula, data=train_df)
lm_fit = lm_model.fit()
mse = np.mean((lm_fit.predict(test_df) - test_df['mpg']) ** 2)
mse_folds[i_degree].append(mse)
    degree.append(i_degree)
    my_formula += ' + I(horsepower ** ' + str(i_degree + 1) + ')'
mse_degree = []
for i_degree in mse_folds.keys():
    mse_degree.append(np.mean(mse_folds[i_degree]))
for i_degree, mse_kfold in zip(degree, mse_degree):
    print('degree: ', i_degree, ', mse_kfold: ', round(mse_kfold, 3))
import sys
sys.path.append('cnoode/chap5/')
import mse_kFoldCV
```

```
degree: 1 , mse_kfold:
                        24.213
degree: 2 , mse_kfold:
                        19.378
degree: 3 , mse_kfold:
                       19.477
degree: 4 , mse_kfold:
                       19.538
degree: 5 , mse_kfold: 19.166
degree: 6 , mse_kfold: 19.183
degree: 7 , mse_kfold:
                       19.157
degree: 8 , mse_kfold:
                        23.247
degree: 9 , mse_kfold:
                        23.258
degree: 10 , mse_kfold: 65.251
```

5.3.4 The Bootstrap

1. Estimating the Accuracy of a Statistic of Interest We will first write a function that takes two inputs, data and index, and calculates the desired statistic α . Then we will repeatedly call this function and store the estimates of α .

```
# alphaBootstrap.py
import numpy as np
import pandas as pd
# from statsmodels import datasets
import statsmodels.formula.api as smf
def alphaEst(returns_df, row_index):
    ''', Assumes returns_df is a return dataframe with two columns of stock returns
    row_index is a list of row indexes to be used in calculation.
    Returns alpha estimate using subset of data defined by row_index.''
    cov_xy = np.cov(returns_df.iloc[row_index], rowvar=False)
    return (cov_xy[1, 1] - cov_xy[0, 1]) / \
(cov_xy[0, 0] + cov_xy[1, 1] - 2 * cov_xy[0, 1])
def bootStrap(my_df, myFunc, sample_size, n_bootstrap, all_res=False):
    ''' Assumes my_df is a dataframe and myFunc is a function that can
    estimate a stastic on my_df. Estimate statistic n_bootstrap times,
    each with a sample of size sample_size.
```

```
Return mean and standard error of statistic.",
    my_stat = []
    for i in range(n_bootstrap):
index = np.random.choice(my_df.shape[0], sample_size)
my_stat.append(myFunc(my_df, index))
    if isinstance(my_stat[0], float):
my_res = {'mean': np.mean(my_stat), 'std. error': np.std(my_stat)}
if all_res:
    my_res['stats'] = my_stat
    elif isinstance(my_stat[0], pd.core.series.Series):
my_stat_dict = {}
for ind in my_stat[0].index:
    my_stat_dict[ind] = []
for i in range(len(my_stat)):
    for key in my_stat_dict.keys():
my_stat_dict[key].append(my_stat[i][key])
my_res = {}
for key in my_stat_dict.keys():
    my_res[key] = {}
    my_res[key]['mean'] = np.mean(my_stat_dict[key])
    my_res[key]['std. error'] = np.std(my_stat_dict[key])
if all_res:
    my_res['stats'] = my_stat
    return my_res
def autoDataCoef(auto_df, row_index):
    '''Assumes auto_df is a dataframe which includes 'mpg' and
    'horsepower' columns. Fit a linear regression model on auto_df.
    Use row_index to create a subset of auto_df. Return regression
    coefficients estimated from subset of auto_df.','
    lm_model = smf.ols('mpg ~ horsepower', data=auto_df.iloc[row_index])
    lm_fit = lm_model.fit()
    return lm_fit.params
def autoDataCoef2(auto_df, row_index):
```

```
''', 'Assumes auto_df is a dataframe which has columns 'mpg' and
    'horsepower'. Fit an OLS regression model with mpg as a
    quadratic function of horsepower. Use subset of auto_df defined
    by row_index. Return regression coefficient estimates. ","
    lm_model = smf.ols('mpg ~ horsepower + I(horsepower ** 2)',
       data=auto_df.iloc[row_index])
    lm_fit = lm_model.fit()
    return lm_fit.params
from statsmodels import datasets
import numpy as np
import sys
sys.path.append('code/chap5/')
from alphaBootstrap import alphaEst, bootStrap
portfolio = datasets.get_rdataset('Portfolio', 'ISLR').data
np.random.seed(911)
alpha_boot = bootStrap(portfolio, alphaEst, sample_size=100, n_bootstrap=1000)
print(alpha_boot)
{'mean': 0.5753949845303641, 'std. error': 0.08938513622277834}
```

2. Estimating the Accuracy of a Linear Regression Model We now use bootstrap method to assess the variability of the estimates for β_0 and β_1 , the intercept and slope terms for the linear regression model that uses horsepower to predict mpg in the Auto data set. We will compare the estimates obtained using the bootstrap to those obtained using the standar formulas for $SE(\hat{\beta}_0)$ and $SE(\hat{\beta}_1)$.

```
from statsmodels import datasets
import statsmodels.formula.api as smf
import numpy as np
import sys
sys.path.append('code/chap5/')
from alphaBootstrap import autoDataCoef, bootStrap
auto = datasets.get_rdataset('Auto', 'ISLR').data
```

np.random.seed(911)

```
mpg_hp_boot = bootStrap(auto, autoDataCoef, sample_size=392, n_bootstrap=1000)
print('Bootstrap results:')
for key in mpg_hp_boot.keys():
    print(key, ':', mpg_hp_boot[key])
print('----')
lm_model = smf.ols('mpg ~ horsepower', data=auto)
lm_fit = lm_model.fit()
print('Regression results:')
print(lm_fit.summary2().tables[1].iloc[:,:4])
Bootstrap results:
Intercept: {'mean': 39.94234375950751, 'std. error': 0.8748453071088308}
horsepower: {'mean': -0.15796112230552348, 'std. error': 0.007526082860287968}
Regression results:
                Coef. Std.Err.
                                                    P>|t|
                                         t
            39.935861 0.717499 55.659841 1.220362e-187
Intercept
horsepower -0.157845 0.006446 -24.489135 7.031989e-81
Finally, we compute the bootstrap standard error estimates and the
standard linear regression estimates that result from fitting the quadratic
model to the Auto data.
Bootstrap results:
Intercept : {'mean': 57.02549325815686, 'std. error': 2.012215071375403}
horsepower: {'mean': -0.46840037414346225, 'std. error': 0.03187991112044731}
I(horsepower ** 2) : {'mean': 0.0012391590913923556, 'std. error': 0.0001152359507
Regression results:
                        Coef. Std.Err.
                                                 t
                                                             P>|t|
Intercept
                    56.900100 1.800427 31.603673 1.740911e-109
horsepower
                    -0.466190 0.031125 -14.978164 2.289429e-40
I(horsepower ** 2)
                     0.001231 0.000122 10.080093
                                                     2.196340e-21
```