A Python Companion to ISLR

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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 $\tt Down$.

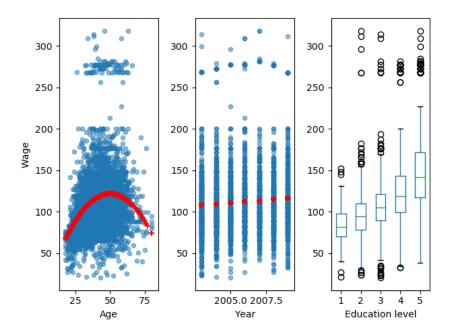


Figure 1: Wage data, which contains income survey information for males from the central Atlantic region of the United States. Left: wage as a function of age. On average, wage increases with age until about 60 years of age, at which point it begins to decline. Center: wage as a function of year. There 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.

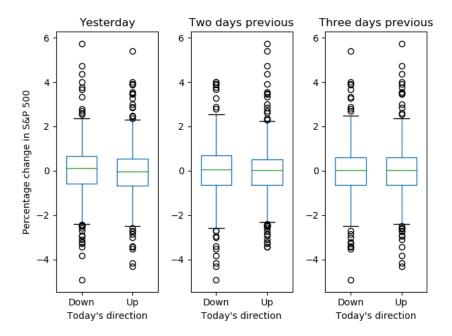


Figure 2: Left: Boxplots of the previous day's percentage change in the S&P 500 index for the days for which the market increased or decreased, obtained from the Smarket data. Center and Right: Same as left panel, but the percentage changes for two and three days previous are shown.

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.

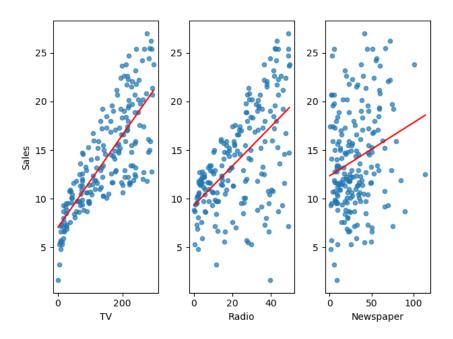


Figure 3: The Advertising data set. The plot displays sales, in thousands of units, as a function of TV, radio, and newspaper budgets, in thousands of dollars, for 200 different markets. In each plot we show the simple least squares fit of sales to that variable. In other words, each red line represents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

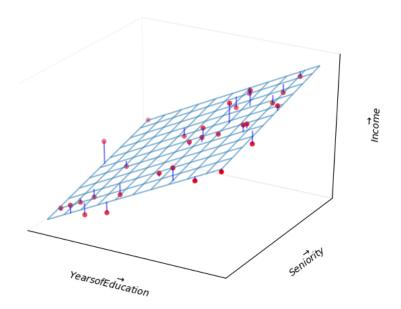


Figure 6: A linear model fit by least squares to the Income data from figure 5. The observations are shown in red, and the blue plane indicates the least squares fit to the data.

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.

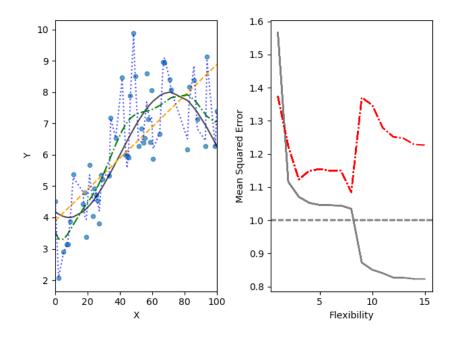


Figure 9: Left: Data simulated from f, shown in black. Three estimates of f are shown: the linear regression line (orange curve), and two smoothing spline fits (blue and green curves). Right: Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed grey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

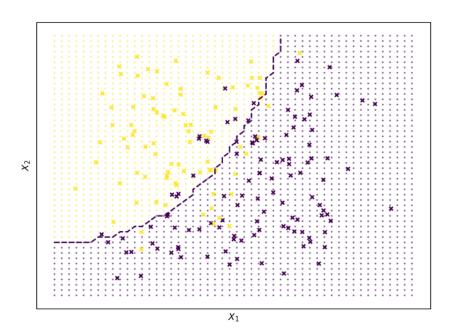


Figure 13: A simulated data set consisting of 200 observations in two groups, indicated in blue and orange. The dashed line represents the Bayes decision boundary. The orange background grid indicates the region in which a test observation will be assigned to the orange class, and blue background grid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

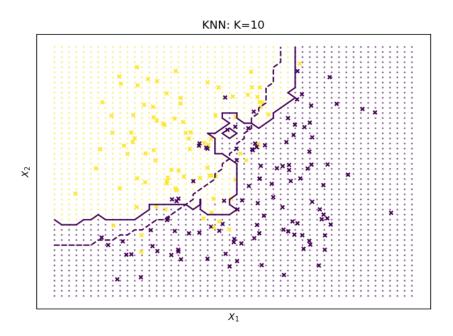


Figure 14: The firm line indicates the KNN decision boundary on the data from figure 13, using K=10. The Bayes decision boundary is shown as a dashed line. The KNN and Bayes decision boundaries are very similar.

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.
                        ]]
```

numpy.random 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 numpy.corrcoef 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]
[[1.
 [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 | year | origin | name |
|---|------|-----------|--------------|----------|--------|---------------------------|
| 0 | 18.0 | 8 | 307.0 | 70 | 1 | chevrolet chevelle malibu |
| 1 | 15.0 | 8 | 350.0 | 70 | 1 | buick skylark 320 |
| 2 | 18.0 | 8 | 318.0 | 70 | 1 | plymouth satellite |
| 3 | 16.0 | 8 | 304.0 | 70 | 1 | amc rebel sst |
| 4 | 17.0 | 8 | 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.

import pandas as pd
from pandas import plotting
```

plotting.scatter_matrix(Auto[['mpg', 'displacement', 'horsepower', 'weight',

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())
```

Auto = pd.read_csv('data/Auto.csv')

'acceleration']])

| | 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.

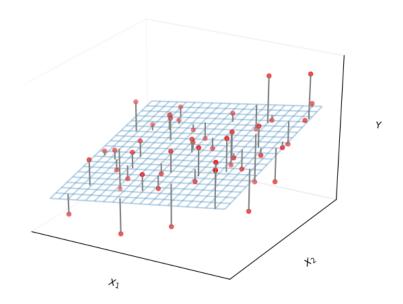


Figure 20: In a three-dimensional setting, with two predictors and one response, the least squares regression line becomes a plane. The plane is chosen to minimize the sum of the squared vertical distances between each observation (shown in red) and the plane.

| | TV | radio | newspaper | 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).

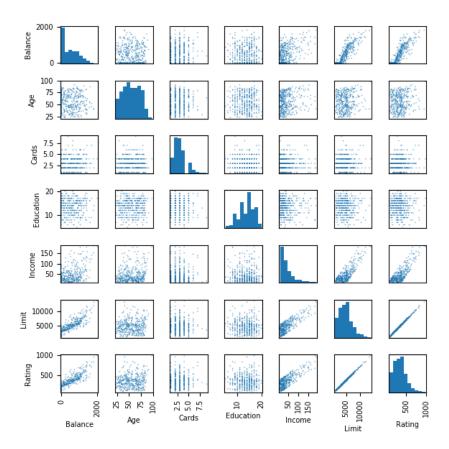


Figure 22: The Credit dataset contains information about balance, age, cards, education, income, limit, and rating for a number of potential customers.

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 qudratic 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

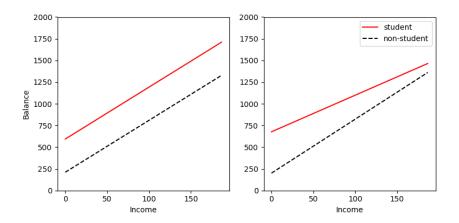


Figure 23: For the Credit data, the least squares lines are shown for prediction of balance from income for students and non-students. Left: There is no interaction between income and student. Right: There is an interaction term between income and students.

| | 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

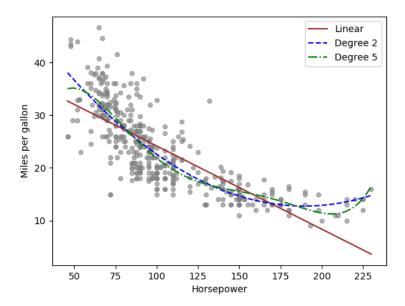


Figure 24: The Auto data set. For a number of cars, mpg and horsepower are shown. The linear regression fit is shown in orange. The linear regression fit for a model that includes first- and second-order terms of horsepower is shown as blue curve. The linear regression fit for a model that includes all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

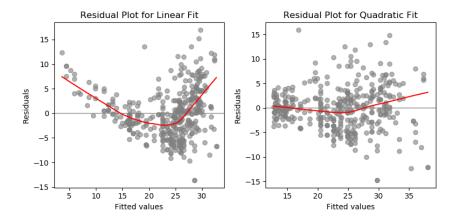


Figure 25: Plots of residuals versus predicted (or fitted) values for the Auto data set. In each plot, the red line is a smooth fit to the residuals, intended to make it easier to identify a trend. Left: A linear regression of mpg on horsepower. A strong pattern in the residuals indicates non-linearity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

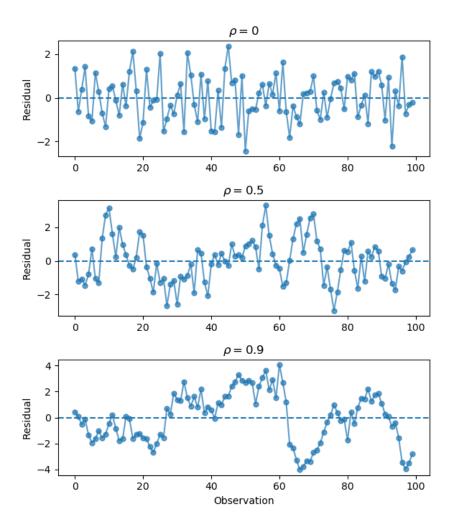


Figure 26: Plots of residuals from simulated time series data sets generated with differeing levels of correlation ρ between error terms for adjacent time points.

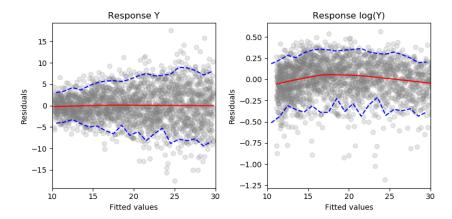


Figure 27: Residual plots. The red line, a smooth fit to the residuals, is intended to make it easier to identify a trend. The blue lines track 5^{th} and 95^{th} percentiles of the residuals, and emphasize patterns. Left: The funnel shape indicates heteroscedasticity. Right: the response has been log 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.

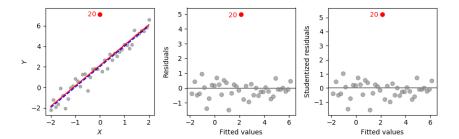


Figure 28: Left: The least squares regression line is shown in red. The regression line after removing the outlier is is shown in blue. Center: The residual plot clearly identifies the outlier. Right: The outlier has a studentized residual of 6; typically we expect values between -3 and 3.

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.

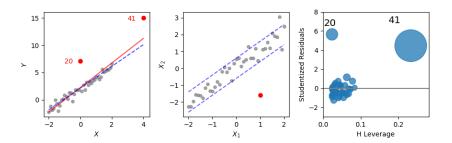


Figure 29: Left: Observation 41 is a high leverage point, while 20 is not. The red line is the fit to all the data, and the blue line is the fit with observation 41 removed. Center: The red observation is not unusual in terms of its X_1 value or its X_2 value, but still falls outside the bulk of the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

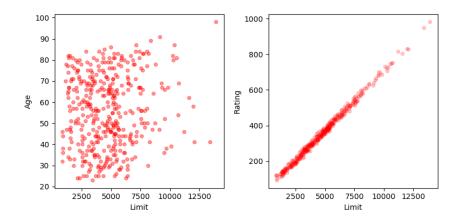


Figure 30: Scatterplots of the observations from the Credit data set. Left: A plot of age versus limit. These two variables not collinear. Right: A plot of rating versus limit. There is high collinearity.

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 upto 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.

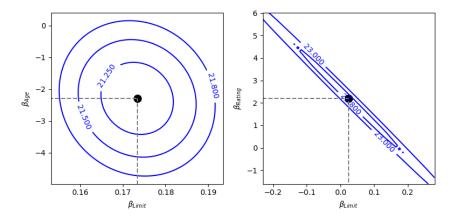


Figure 31: Contour plots for the RSS values as a function of the parameters β for various regressions involving the Credit data set. In each plot, the black dots represent the coefficient values corresponding to the minimum RSS. Left: A contour plot of RSS for the regression of balance onto age and limit. 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.

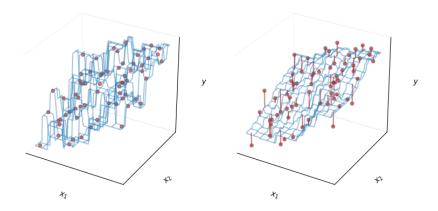


Figure 32: Plots of $\hat{f}(X)$ using KNN regression on two-dimensional data set with 64 observations (brown dots). Left: K=1 results in a rough step function fit. Right: K=9 produces a much smoother fit.

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.

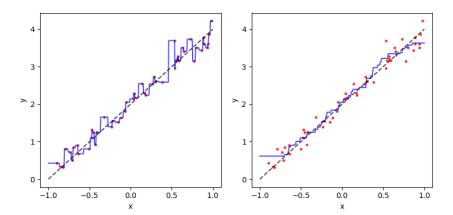


Figure 33: Plots of $\hat{f}(X)$ using KNN regression on a one-dimensional data set with 50 observations. The true relationship is given by the black dashed line. Left: The blue curve corresponds to K=1 and interpolates (i.e., passes directly through) training data. Right: The blue curve corresponds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

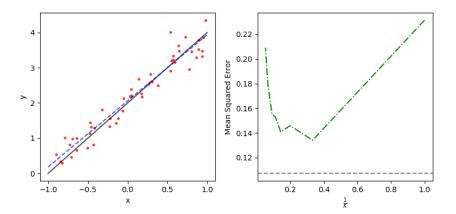


Figure 34: The same data set shown in figure 33 is investigated further. Left: The blue dashed line is the least squares fit to the data. Since f(X) is in fact linear (displayed in black line), the least squares regression line provides a very good estimate of f(X). Right: The dashed horizontal line 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.

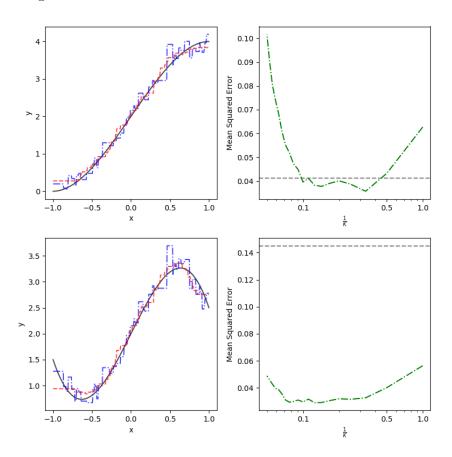


Figure 35: Top Left: In a setting with a slightly non-linear relationship between X and Y (solid black line), the KNN fits with K=1 (blue) and K=9 (red) are displayed. Top Right: For the slightly non-linear data,the test set MSE for least squares regression (horizontal) and KNN with various values of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

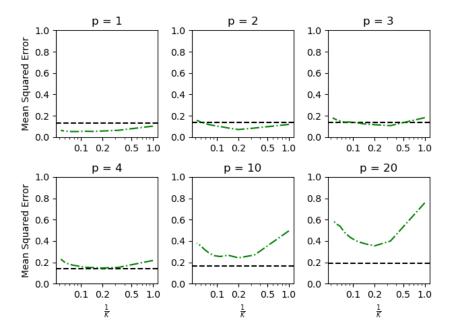


Figure 36: Test MSE for linear regressions (black horizontal lines) and KNN (green curves) as the number of variables p increases. The true function is non-linear in the first variable, as in the lower panel in figure 35, and does not depend upon the additional variables. The performance of linear regression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

3.6 Lab: Linear Regression

It is possible to call R from Python and vice versa.