

18-Regression-II-Logistic

November 11, 2016

1 Logistic Regression

So far we have seen linear regression: a continuous valued observation is estimated as linear (or affine) function of the independent variables.

Today we will look at the following situation.

Imagine that you are observing a binary variable – a 0/1 value.

That is, these could be pass/fail, admit/reject, Democrat/Republican, etc.

You believe that there is some **probability** of observing a 1, and that probability is a function of certain independent variables.

So the key properties of a problem that make it appropriate for logistic regression are:

- What you can observe is a **categorical** variable
- What you want to estimate is a **probability** of seeing a particular value of the categorical variable.

1.1 What is the probability I will be admitted to Grad School?

From <http://www.ats.ucla.edu/stat/r/dae/logit.htm>:

A researcher is interested in how variables, such as *GRE* (Graduate Record Exam scores), *GPA* (grade point average) and prestige of the undergraduate institution affect admission into graduate school. The response variable, admit/don't admit, is a binary variable.

There are three predictor variables: **gre**, **gpa** and **rank**. We will treat the variables *gre* and *gpa* as continuous. The variable *rank* takes on the values 1 through 4. Institutions with a rank of 1 have the highest prestige, while those with a rank of 4 have the lowest.

```
In [3]: # data source: http://www.ats.ucla.edu/stat/data/binary.csv
df = pd.read_csv('data/ats-admissions.csv')
df.head(10)
```

```
Out[3]:
```

	admit	gre	gpa	rank
0	0	380	3.61	3
1	1	660	3.67	3
2	1	800	4.00	1
3	1	640	3.19	4
4	0	520	2.93	4
5	1	760	3.00	2
6	1	560	2.98	1

```

7      0  400  3.08    2
8      1  540  3.39    3
9      0  700  3.92    2

```

```
In [4]: df.describe()
```

```

Out[4]:
          admit          gre          gpa          rank
count  400.000000  400.000000  400.000000  400.000000
mean     0.317500  587.700000    3.389900    2.485000
std     0.466087  115.516536    0.380567    0.944466
min     0.000000  220.000000    2.260000    1.000000
25%     0.000000  520.000000    3.130000    2.000000
50%     0.000000  580.000000    3.395000    2.000000
75%     1.000000  660.000000    3.670000    3.000000
max     1.000000  800.000000    4.000000    4.000000

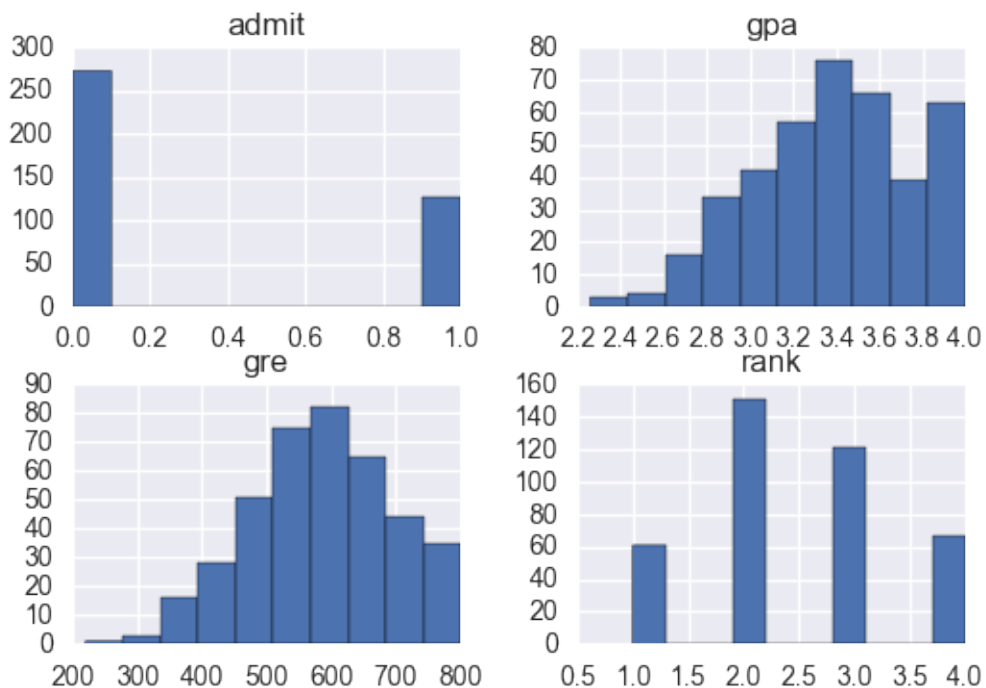
```

```
In [5]: df.hist()
```

```

Out[5]: array([[<matplotlib.axes._subplots.AxesSubplot object at 0x10475e400>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x116380208>],
               [<matplotlib.axes._subplots.AxesSubplot object at 0x1163b6828>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x1164081d0>]], dt

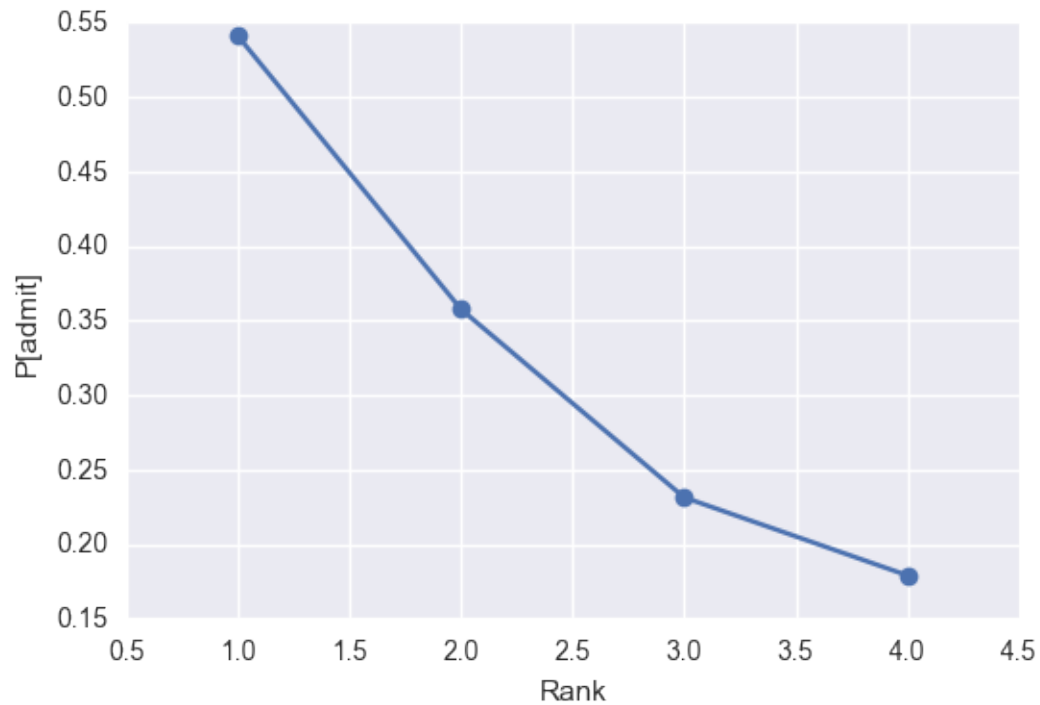
```



Let's look at how each independent variable affects admission probability.

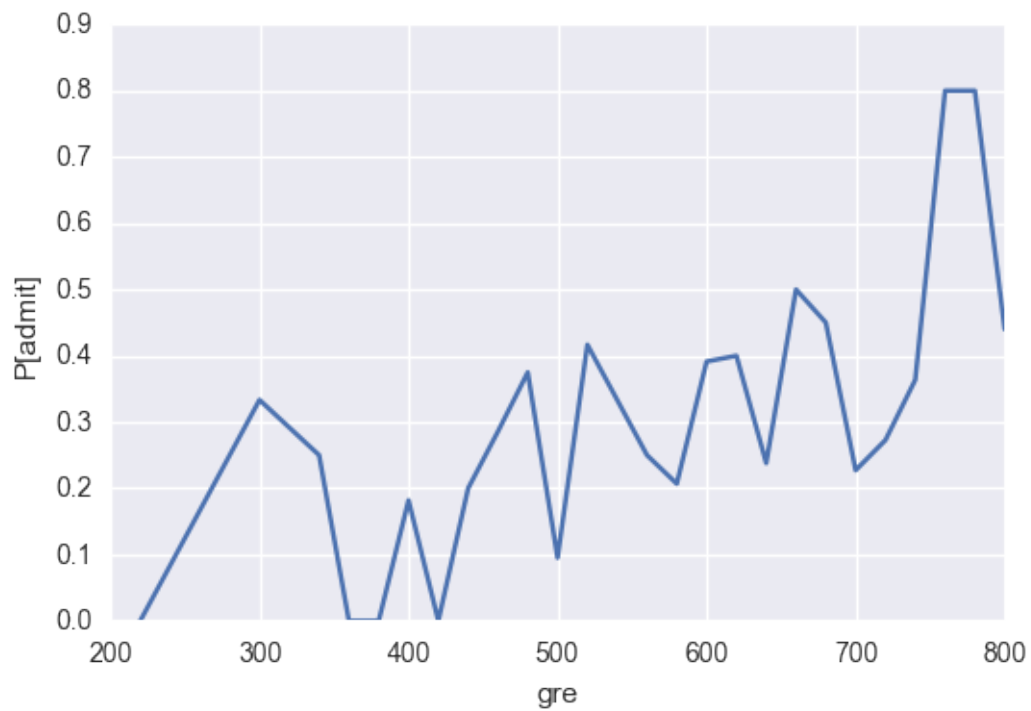
First, **rank**:

```
In [6]: plt.plot(df.groupby('rank').mean()['admit'],'o-')
plt.xlabel('Rank')
plt.xlim([0.5,4.5])
_=plt.ylabel('P[admit]')
```



Next, **GRE**:

```
In [7]: plt.plot(df.groupby('gre').mean()['admit'])
plt.xlabel('gre')
_=plt.ylabel('P[admit]')
```



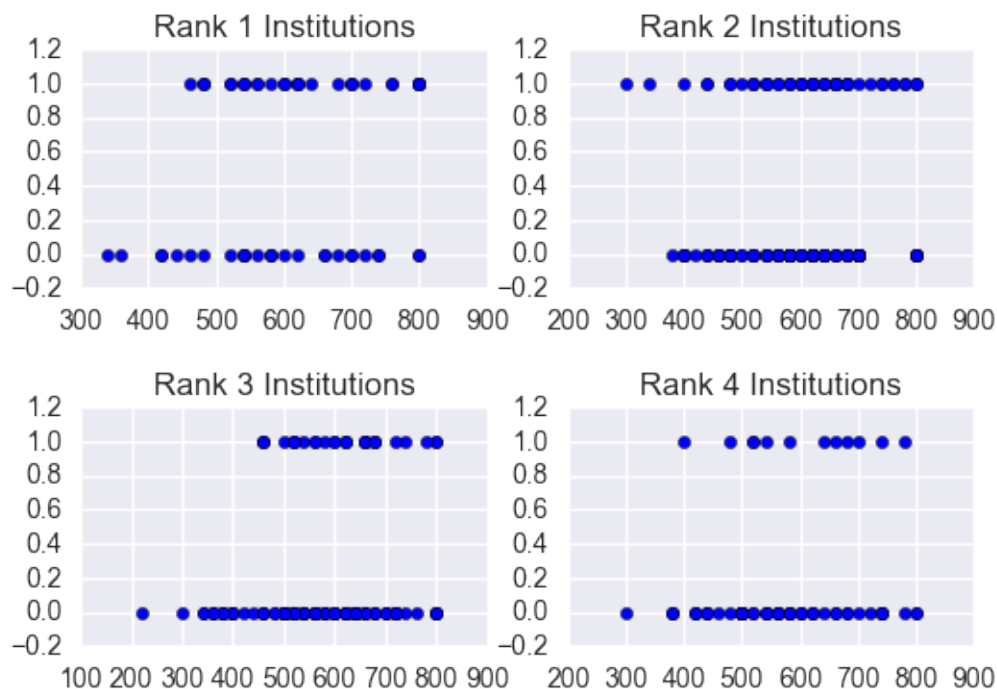
Finally, **GPA** (for this visualization, we aggregate GPA into 10 bins):

```
In [8]: bins = np.linspace(df.gpa.min(), df.gpa.max(), 10)
groups = df.groupby(np.digitize(df.gpa, bins))
plt.plot(bins, groups.admit.mean())
plt.xlabel('gpa')
_=plt.ylabel('P[admit]')
```



Furthermore, we can see that the independent variables are strongly correlated:

```
In [9]: df1 = df[df['rank']==1]
        df2 = df[df['rank']==2]
        df3 = df[df['rank']==3]
        df4 = df[df['rank']==4]
        plt.subplot(221)
        plt.scatter(df1['gre'], df1['admit'])
        plt.title('Rank 1 Institutions')
        plt.subplot(222)
        plt.title('Rank 2 Institutions')
        plt.scatter(df2['gre'], df2['admit'])
        plt.subplot(223)
        plt.scatter(df3['gre'], df3['admit'])
        plt.title('Rank 3 Institutions')
        plt.subplot(224)
        plt.title('Rank 4 Institutions')
        plt.scatter(df4['gre'], df4['admit'])
        plt.subplots_adjust(hspace=0.5)
```



1.2 Logistic Regression

Logistic regression is concerned with estimating a **probability**.

However, all that is available are categorical observations, which we will code as 0/1.

That is, these could be pass/fail, admit/reject, Democrat/Republican, etc.

Now, a linear function like $\alpha + \beta x$ cannot be used to predict probability directly, because the linear function takes on all values (from $-\infty$ to $+\infty$), and probability only ranges over $(0, 1)$.

However, there is a transformation of probability that works: it is called **log-odds**.

For any probability p , the **odds** is defined as $p/(1 - p)$. Notice that odds vary from 0 to ∞ , and odds < 1 indicates that $p < 1/2$.

Now, there is a good argument that to fit a linear function, instead of using odds, we should use log-odds. That is simply $\log p/(1 - p)$.

So, logistic regression does the following: it does a linear regression of $\alpha + \beta x$ against $\log p/(1 - p)$.

That is, it fits:

$$\alpha + \beta x = \log \frac{p(x)}{1 - p(x)}$$

$$e^{\alpha + \beta x} = \frac{p(x)}{1 - p(x)}$$

$$e^{\alpha + \beta x}(1 - p(x)) = p(x)$$

$$e^{\alpha + \beta x} = p(x) + p(x)e^{\alpha + \beta x}$$

$$\frac{e^{\alpha+\beta x}}{1+e^{\alpha+\beta x}} = p(x)$$

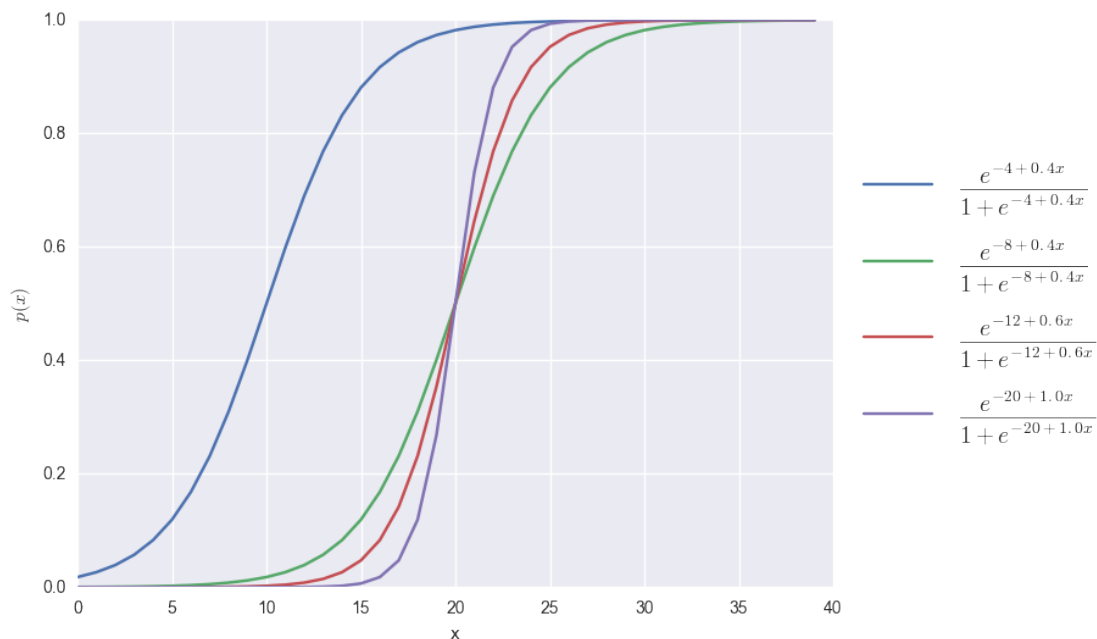
So, logistic regression fits a probability of the following form:

$$p(x) = P(y = 1 | x) = \frac{e^{\alpha+\beta x}}{1+e^{\alpha+\beta x}}$$

This is a sigmoid function; when $\beta > 0$, $x \rightarrow \infty$, then $p(x) \rightarrow 1$ and when $x \rightarrow -\infty$, then $p(x) \rightarrow 0$.

```
In [10]: alphas = [-4, -8, -12, -20]
betas = [0.4, 0.4, 0.6, 1]
x = np.arange(40)
fig = plt.figure(figsize=(8, 6))
ax = plt.subplot(111)

for i in range(len(alphas)):
    a = alphas[i]
    b = betas[i]
    y = np.exp(a+b*x) / (1+np.exp(a+b*x))
    plt.plot(x,y, label=r"$\frac{e^{\%d + \%3.1fx}}{1+e^{\%d + \%3.1fx}}$" % (a, b))
plt.xlabel('x')
plt.ylabel('$p(x)$')
_=ax.legend(loc='center left', bbox_to_anchor=(1, 0.5), prop={'size': 20})
```



Parameter β controls how fast $p(x)$ raises from 0 to 1
The value of $-\alpha/\beta$ shows the value of x for which $p(x) = 0.5$

Another interpretation of α is that it gives the **base rate** – the unconditional probability of a 1. That is, if you knew nothing about a particular data item, then $p(x) = 1/(1 + e^{-\alpha})$.

The function $f(x) = \log(x/(1 - x))$ is called the **logit** function.

So a compact way to describe logistic regression is that it finds regression coefficients α, β to fit:

$$\text{logit}(p(x)) = \log\left(\frac{p(x)}{1 - p(x)}\right) = \alpha + \beta x$$

Note also that the **inverse** logit function is:

$$\text{logit}^{-1}(x) = \frac{e^x}{1 + e^x}$$

Somewhat confusingly, this is called the **logistic** function.

So, the best way to think of logistic regression is that we compute a linear function:

$$\alpha + \beta x$$

and then “map” that to a probability using the logit^{-1} function:

$$\frac{e^{\alpha + \beta x}}{1 + e^{\alpha + \beta x}}$$

1.3 Logistic vs Linear Regression

Let’s take a moment to compare linear and logistic regression.

In **Linear regression** we fit

$$y_i = \alpha + \beta x_i + \epsilon_i.$$

We do the fitting by minimizing the sum of squared error ($\|\epsilon\|$). This can be done in closed form.

(Recall that the closed form is found by geometric arguments, or by calculus).

Now, if ϵ_i comes from a normal distribution with mean zero and some fixed variance,

then minimizing the sum of squared error is exactly the same as finding the maximum likelihood of the data with respect to the probability of the errors.

So, in the case of linear regression, it is a lucky fact that the **MLE** of α and β can be found by a **closed-form** calculation.

In **Logistic regression** we fit

$$\text{logit}(p(x_i)) = \alpha + \beta x_i.$$

with $\Pr(y_i = 1 \mid x_i) = p(x_i)$.

How should we choose parameters?

Here too, we use Maximum Likelihood Estimation of the parameters.

That is, we choose the parameter values that maximize the likelihood of the data given the model.

$$\Pr(y_i \mid x_i) = \begin{cases} \text{logit}^{-1}(\alpha + \beta x_i) & \text{if } y_i = 1 \\ 1 - \text{logit}^{-1}(\alpha + \beta x_i) & \text{if } y_i = 0 \end{cases}$$

We can write this as a single expression:

$$\Pr(y_i | x_i) = \text{logit}^{-1}(\alpha + \beta x_i)^{y_i} (1 - \text{logit}^{-1}(\alpha + \beta x_i))^{1-y_i}$$

We then use this to compute the **likelihood** of parameters α, β :

$$L(\alpha, \beta | x_i, y_i) = \text{logit}^{-1}(\alpha + \beta x_i)^{y_i} (1 - \text{logit}^{-1}(\alpha + \beta x_i))^{1-y_i}$$

which is a function that we can maximize via various kinds of gradient descent.

1.4 Logistic Regression In Practice

So, in summary, we have:

Input pairs (x_i, y_i)

Output parameters $\hat{\alpha}$ and $\hat{\beta}$ that maximize the likelihood of the data given these parameters for the logistic regression model.

Method Maximum likelihood estimation, obtained by gradient descent.

The standard package will give us a correlation coefficient (a β_i) for each independent variable (feature).

If we want to include a constant (ie, α) we need to add a column of 1s (just like in linear regression).

```
In [11]: df['intercept'] = 1.0
         train_cols = df.columns[1:]
         train_cols

Out[11]: Index(['gre', 'gpa', 'rank', 'intercept'], dtype='object')

In [12]: logit = sm.Logit(df['admit'], df[train_cols])

         # fit the model
         result = logit.fit()
```

```
Optimization terminated successfully.
Current function value: 0.574302
Iterations 6
```

```
In [13]: result.summary()
```

```
Out[13]: <class 'statsmodels.iolib.summary.Summary'>
        """
```

```

                                Logit Regression Results
=====
Dep. Variable:                  admit    No. Observations:
Model:                          Logit    Df Residuals:
Method:                          MLE     Df Model:
Date:                            Thu, 10 Nov 2016    Pseudo R-squ.:          0.0
Time:                            10:43:16    Log-Likelihood:         -22
converged:                       True     LL-Null:              -24
                                LLR p-value:          8.207
```

```
=====
              coef      std err          z      P>|z|      [95.0% Conf. Int.]
-----
gre           0.0023      0.001      2.101      0.036      0.000      0.000
gpa           0.7770      0.327      2.373      0.018      0.135      0.135
rank        -0.5600      0.127     -4.405      0.000     -0.809     -0.809
intercept   -3.4495      1.133     -3.045      0.002     -5.670     -5.670
=====
"""
```

Notice that all of our independent variables are considered significant (no confidence intervals contain zero).

1.5 Using the Model

Note that by fitting a model to the data, we can make predictions for inputs that were never seen in the data.

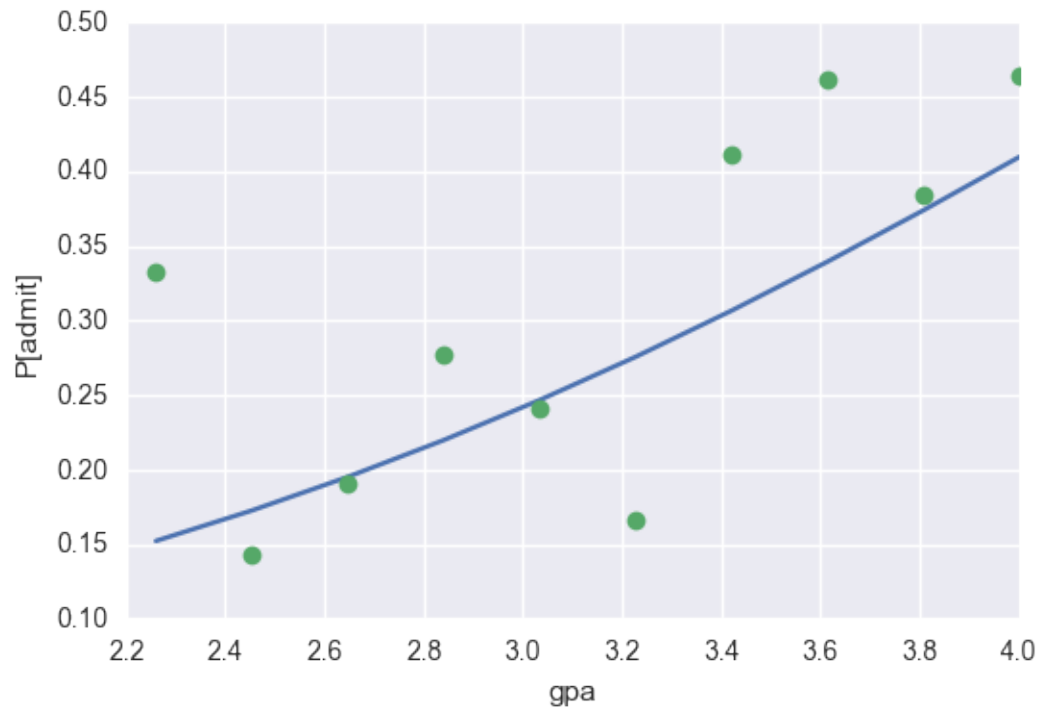
Furthermore, we can make a prediction of a probability for cases where we don't have enough data to estimate the probability directly – e.g, for specific parameter values.

Let's see how well the model fits the data.

We have three independent variables, so in each case we'll use average values for the two that we aren't evaluating.

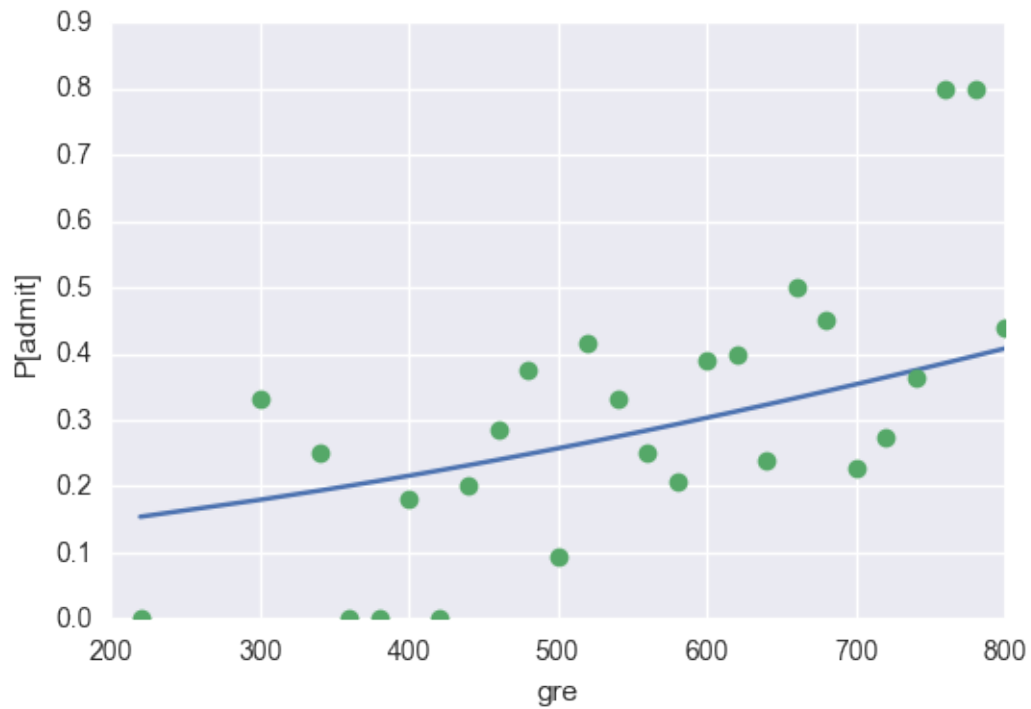
GPA:

```
In [14]: bins = np.linspace(df.gpa.min(), df.gpa.max(), 10)
         groups = df.groupby(np.digitize(df.gpa, bins))
         prob = [result.predict([600, b, 2.5, 1.0]) for b in bins]
         plt.plot(bins, prob)
         plt.plot(bins, groups.admit.mean(), 'o')
         plt.xlabel('gpa')
         plt.ylabel('P[admit]')
```



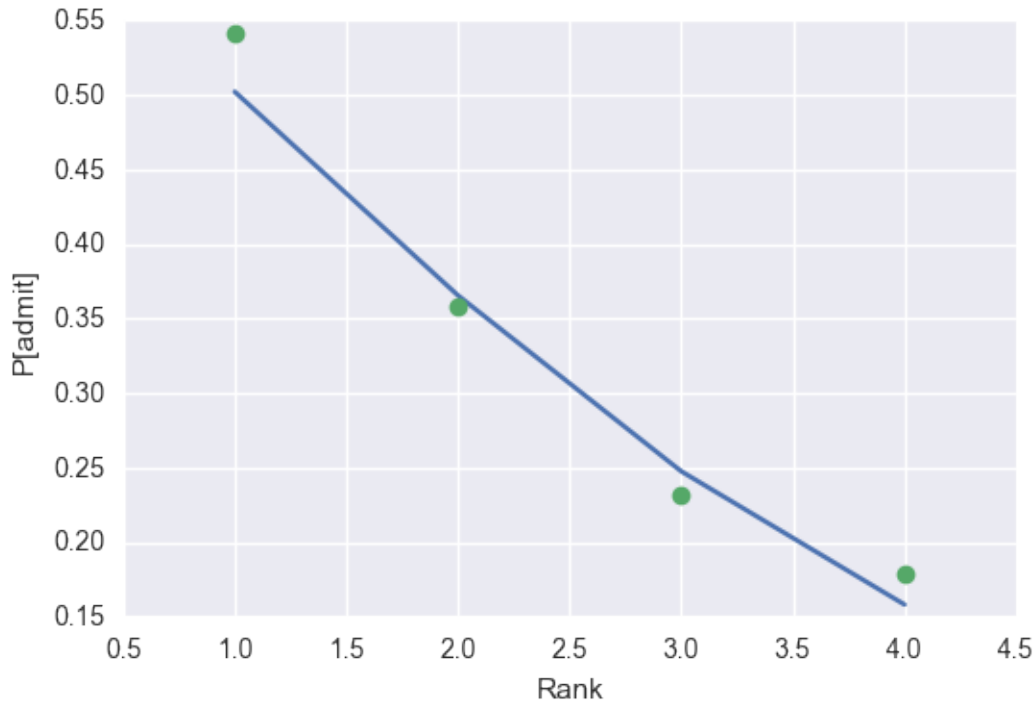
GRE Score:

```
In [15]: prob = [result.predict([b, 3.4, 2.5, 1.0]) for b in sorted(df.gre.unique())
plt.plot(sorted(df.gre.unique()), prob)
plt.plot(df.groupby('gre').mean()['admit'], 'o')
plt.xlabel('gre')
_=plt.ylabel('P[admit]')
```



Institution Rank:

```
In [16]: prob = [result.predict([600, 3.4, b, 1.0]) for b in range(1,5)]
plt.plot(range(1,5), prob)
plt.plot(df.groupby('rank').mean()['admit'], 'o')
plt.xlabel('Rank')
plt.xlim([0.5, 4.5])
_=plt.ylabel('P[admit]')
```



1.6 Logistic Regression in Perspective

At the start of lecture I emphasized that logistic regression is concerned with estimating a **probability** model from **discrete** (0/1) data.

However, it may well be the case that we want to do something with the probability that amounts to **classification**.

For example, we may classify data items using a rule such as “Assign item x_i to Class 1 if $p(x_i) > 0.5$ ”.

For this reason, logistic regression could be considered a classification method.

In fact, that is what we did with Naive Bayes – we used it to estimate something like a probability, and then chose the class with the maximum value to create a classifier.

Let’s use our logistic regression as a classifier.

We want to ask whether we can correctly predict whether a student gets admitted to graduate school.

Let’s separate our training and test data:

```
In [17]: X_train, X_test, y_train, y_test = cross_validation.train_test_split(
        df[train_cols], df['admit'],
        test_size=0.4, random_state=1)
```

Now, there are some standard metrics used when evaluating a binary classifier.

Let’s say our classifier is outputting “yes” when it thinks the student will be admitted.

There are four cases: * Classifier says “yes”, and student **is** admitted: **True Positive**. * Classifier says “yes”, and student **is not** admitted: **False Positive**. * Classifier says “no”, and student **is** admitted: **False Negative**. * Classifier says “no”, and student **is not** admitted: **True Negative**.

Precision is the fraction of “yes”es that are correct:

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

Recall is the fraction of admits that we say “yes” to:

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

```
In [18]: def evaluate(y_train, X_train, y_test, X_test, threshold):
    logit = sm.Logit(y_train, X_train)
    result = logit.fit(dispatch=False)

    truePositives = falsePositives = trueNegatives = falseNegatives = 0
    for x, y, in zip(X_test.values, y_test):
        yhat = result.predict(x)
        if y==1 and yhat > threshold:
            truePositives += 1
        elif y==1:
            falseNegatives += 1
        elif yhat > threshold:
            falsePositives += 1
        else:
            trueNegatives +=1

    if (truePositives + falsePositives) == 0:
        precision = 0
    else:
        precision = truePositives / (truePositives + falsePositives)

    if (truePositives + falseNegatives) == 0:
        recall = 0
    else:
        recall = truePositives / (truePositives + falseNegatives)

    return precision, recall

precision, recall = evaluate(y_train, X_train, y_test, X_test, 0.5)

print('\nPrecision: {:.3f}, Recall: {:.3f}'.format(precision, recall))
```

Precision: 0.586, Recall: 0.340

Now, let's get a sense of average accuracy:

```
In [19]: PR = []
    for i in range(20):
```

```

X_train, X_test, y_train, y_test = cross_validation.train_test_split(
    df[train_cols], df['admit'],
    test_size=0.4)
PR.append(evaluate(y_train, X_train, y_test, X_test, 0.5))

In [20]: avgPrec = np.mean([f[0] for f in PR])
        avgRec = np.mean([f[1] for f in PR])
        print('\nAverage Precision: {:.3f}, Average Recall: {:.3f}'.format(avgPrec, avgRec))

```

Average Precision: 0.614, Average Recall: 0.207

Sometimes we would like a single value that describes the overall performance of the classifier. For this, we take the harmonic mean of precision and recall, called **F1 Score**:

$$\text{F1 Score} = 2 \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

Using this, we can evaluate other settings for the threshold.

```

In [21]: def evalThresh(df, thresh):
        PR = []
        for i in range(20):
            X_train, X_test, y_train, y_test = cross_validation.train_test_split(
                df[train_cols], df['admit'],
                test_size=0.4)
            PR.append(evaluate(y_train, X_train, y_test, X_test, thresh))
        avgPrec = np.mean([f[0] for f in PR])
        avgRec = np.mean([f[1] for f in PR])
        return 2 * (avgPrec * avgRec) / (avgPrec + avgRec), avgPrec, avgRec

        tvals = np.linspace(0.05, 0.95, 50)
        flvals = [evalThresh(df, tval)[0] for tval in tvals]

In [22]: plt.plot(tvals, flvals)
        plt.ylabel('F1 Score')
        _=plt.xlabel('Threshold for Classification')

```



Based on this plot, we can say that the best classification threshold appears to be around 0.3, where precision and recall are:

```
In [23]: F1, Prec, Rec = evalThresh(df, 0.3)
         print('Best Precision: {:.0.3f}, Best Recall: {:.0.3f}'.format(Prec, Rec))
```

```
Best Precision: 0.403, Best Recall: 0.681
```

The example here is based on <http://blog.yhathq.com/posts/logistic-regression-and-python.html> where you can find additional details.