introduction-to-regression-analysis

April 25, 2019

1 Regression analysis of medical data

Antti Honkela, antti.honkela@helsinki.fi

We have earlier done linear regression using scikit-learn. In this project work, however, we will use the Statsmodels library. This is because Statsmodels has better statistical tools. In addition, it works better with Pandas' DataFrames, since it can specify the relation between the dependent and independent variables using a formula notation of column names of a DataFrame. Below is an example of a formula:

```
formula = "Y ~ X1 + X2"
```

So, the formula is given as a string where the on the left side of the ~ character is the dependent variable, and on the right side the independent variables, separated using the + character. In this example the variable names `Y`, `X1`, and `X2` refer to columns of a DataFrame.

```
In [3]: import numpy as np
        import matplotlib.pyplot as plt
        import statsmodels
        import statsmodels.api as sm
        import statsmodels.formula.api as smf
        # plots a line given an intercept and a slope
        from statsmodels.graphics.regressionplots import abline_plot
        import pandas as pd
```

2 Multi-variable linear regression

Topics: - Multiple linear regression - Use of background variables to rectify regression - Interactions between variables - Choosing variables - Interpretation of estimation results

Multi-variable linear regression is used to model phenomena that depend on multiple variables. It can be used to adjust the model to consider confounding variables. It can also be used to recognize factors that have significant effect on a phenomenon.

Learning targets: - Fit multi-variable linear regression models in Python - Rectify regression models with background variables, and analyse the rectified models - Understand the principle of variable choosing - Understand most important restrictions of multiple linear regression models

Simple linear regression model is

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

where

- y_i is the explained variable
- x_i is the explanatory variable
- β is the regression coefficient

- α is the constant term (intercept)
- ϵ_i is the residual.

Multi-variable linear regression model (or multiple liner regression model) is

$$y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$$

- y_i is the explained variable
- x_{ij} are the explanatory variables $j = 1, \ldots, p$

- β_j are the regression coefficients
- α is the constant term (intercept)
- ϵ_i is the residual.

The data can be represented as a design matrix that has variables as columns and observations as rows.

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

The whole regression model in a matrix form is

$$y = \alpha \mathbf{1} + X\beta + \mathbf{ffl}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \alpha \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} + \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \mathbf{ffl}$$

$$y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$$

Or equivalently

$$y = \begin{pmatrix} 1 & X \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} + \mathbf{ffl}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix} + \mathbf{ffl}$$

$$y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$$

Or as Python expression:

```
y == np.concatenate([np.ones((len(x), 1)), X], axis=1) @ fit.params
```

2.0.1 An example using the Framingham Heart study

Data from the Framingham Heart study. In 1948, the study was initiated to identify the common factors or characteristics that contribute to CVD by following its development over time in group of participants who had not yet developed overt symptoms of CVD or suffered a heart attack or stroke. The researchers recruited 5,209 men and women between the ages of 30 and 62 from the town of Framingham, Massachusetts. Every two years, a series of extensive physical examinations and lifestyle interviews were conducted. This data set is subset of the Framingham Heart study data. The data is stored as 14 columns. Each row represents a single subject.

```
In [4]: # Load the data
        fram = pd.read_csv('fram.txt', sep='\t')
        fram.head()
```

```
Out[4]:      ID     SEX  AGE  FRW  SBP  SBP10  DBP  CHOL  CIG  CHD YRS_CHD  DEATH  \
        0  4988  female   57  135  186    NaN  120   150    0    1     pre      7
        1  3001  female   60  123  165    NaN  100   167   25    0      16     10
        2  5079  female   54  115  140    NaN   90   213    5    0       8      8
        3  5162  female   52  102  170    NaN  104   280   15    0      10      7
        4  4672  female   45   99  185    NaN  105   326   20    0       8     10

           YRS_DTH    CAUSE
        0       11  unknown
        1       17  unknown
        2       13  unknown
        3       11  unknown
        4       17  unknown
```

ID	Explanation
SEX	Gender
AGE	Age at the start of the study
FRW	Weight in relation to groups median
SBP	Systolic Blood Pressure
DBP	Diastolic Blood Pressure
CHOL	Cholestherol level
CIG	Smoking (cigarets per day)

As an example, let's predict the systolic blood pressure using the weight.

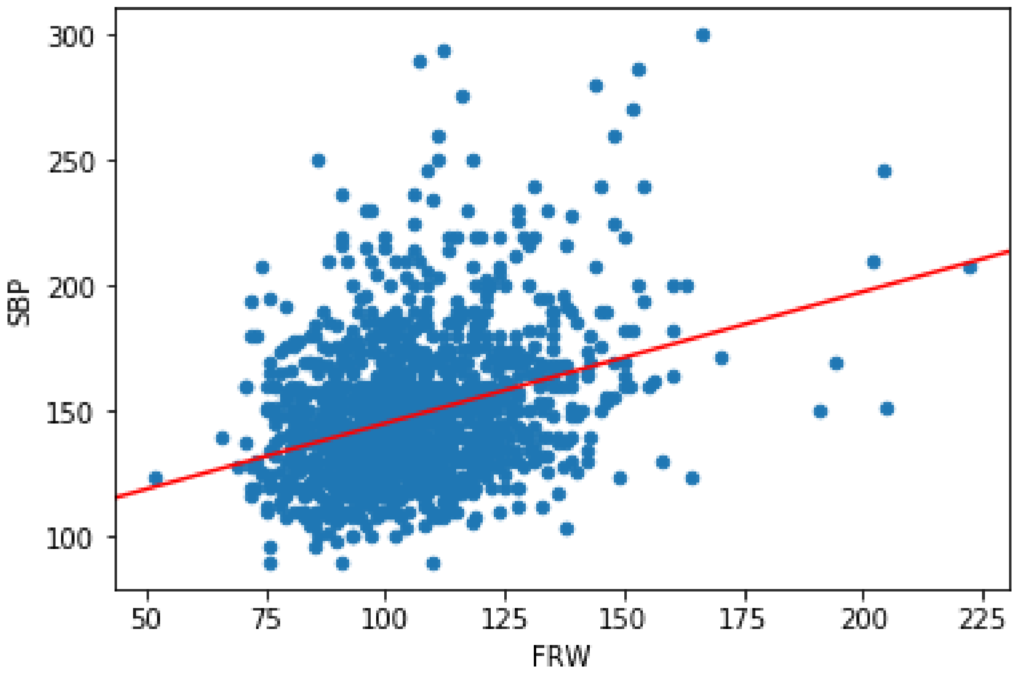
```
In [5]: fit = smf.ols('SBP ~ FRW', data=fram).fit()
        print(fit.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.110
Model:                            OLS   Adj. R-squared:                  0.110
Method:                 Least Squares   F-statistic:                     172.5
```

```
Date:                Thu, 25 Apr 2019   Prob (F-statistic):          3.18e-37
Time:                        22:08:31   Log-Likelihood:               -6542.3
No. Observations:                1394   AIC:                        1.309e+04
Df Residuals:                    1392   BIC:                        1.310e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept     92.8658      4.264     21.778      0.000      84.501     101.231
FRW            0.5241      0.040     13.132      0.000       0.446       0.602
==============================================================================
Omnibus:                      338.464   Durbin-Watson:                   1.756
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              883.998
Skew:                           1.271   Prob(JB):                    1.10e-192
Kurtosis:                       5.959   Cond. No.                         643.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

```
In [6]: fram.plot.scatter("FRW", "SBP")
        #abline(results.params.Intercept, results.params.FRW, col="red")
        abline_plot(intercept=fit.params.Intercept, slope=fit.params.FRW,
                    ax=plt.gca(), color="red");
```



Next we rectify the model using background variables.

Assumptions of a regression model: 1. Relevance of data to the research question 2. Linearity and additivity 3. Independence of residuals 4. Constancy of variance of residuals 5. Normal distribution of residuals

Do these hold now?

In multiple-variable regression we add the background variables as explanators. Note: this rectification is linear an additive. In principle one should include all background variables, but estimation using too many variable can be unreliable.

Let's first consider a binary variable (gender).

```
In [7]: # Incorporate the gender
        fit=smf.ols('SBP ~ FRW + SEX', data=fram).fit()
        print(fit.summary())
```

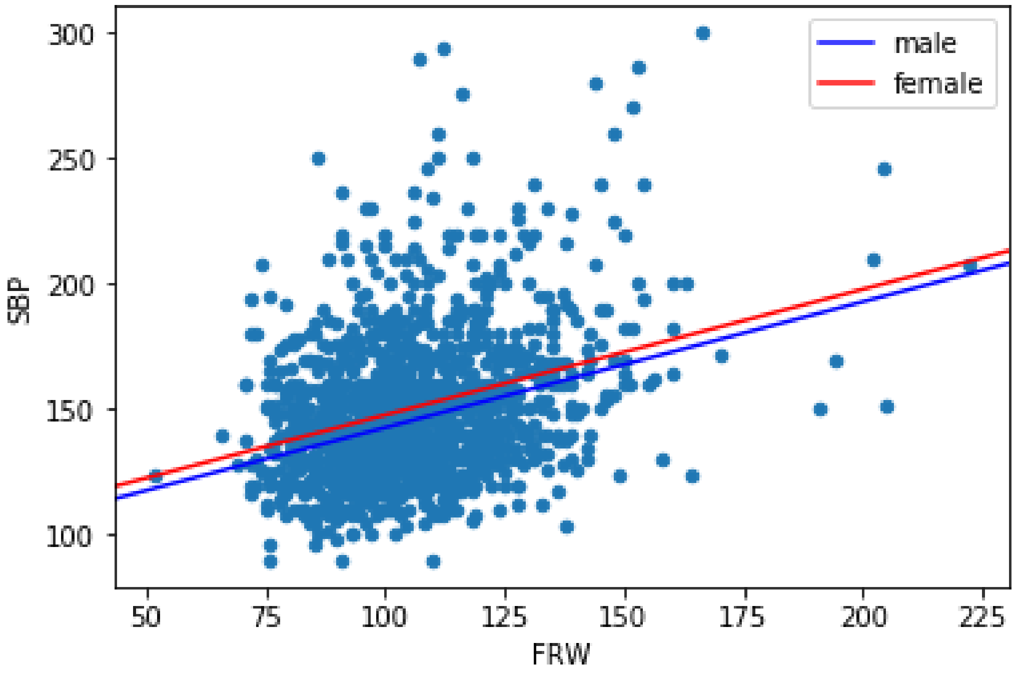
```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.118
Model:                            OLS   Adj. R-squared:                  0.117
Method:                 Least Squares   F-statistic:                     92.94
Date:                Thu, 25 Apr 2019   Prob (F-statistic):           1.31e-38
Time:                        22:08:31   Log-Likelihood:                -6536.3
No. Observations:                1394   AIC:                         1.308e+04
Df Residuals:                    1391   BIC:                         1.309e+04
Df Model:                           2
Covariance Type:            nonrobust
===============================================================================
                  coef    std err          t      P>|t|      [0.025      0.975]
-------------------------------------------------------------------------------
Intercept      97.6608      4.466     21.866      0.000      88.899     106.422
SEX[T.male]    -4.9701      1.432     -3.470      0.001      -7.780      -2.161
FRW             0.5010      0.040     12.431      0.000       0.422       0.580
==============================================================================
Omnibus:                      330.964   Durbin-Watson:                   1.768
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              851.938
Skew:                           1.249   Prob(JB):                    1.01e-185
Kurtosis:                       5.902   Cond. No.                         680.
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

Next we visualize men separately from women.

```
In [8]: fram.plot.scatter("FRW", "SBP")
        int1 = fit.params.Intercept + fit.params["SEX[T.male]"]
        int2 = fit.params.Intercept
        slope=fit.params.FRW
```

```
abline_plot(intercept=int1, slope=slope, ax=plt.gca(), color="blue", label="male")
abline_plot(intercept=int2, slope=slope, ax=plt.gca(), color="red", label="female")
plt.legend();
```



The previous model acknowledged the gender in the intercept, but not in the slope. We improve the model by adding an *interaction term* `FRW:SEX`. Interaction is the product of the two variables. (Note that in these dependence formulas `A * B` is an abbreviation for `A + B + A:B`. The `*` character is not often used in the formulas.)

```
In [9]: # Include both gender and its interaction with the weight
        fit2=smf.ols('SBP ~ FRW + SEX + FRW:SEX', data=fram).fit()
        print(fit2.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.118
Model:                            OLS   Adj. R-squared:                  0.116
Method:                 Least Squares   F-statistic:                     61.92
Date:                Thu, 25 Apr 2019   Prob (F-statistic):           1.42e-37
Time:                        22:08:32   Log-Likelihood:                -6536.3
No. Observations:                1394   AIC:                         1.308e+04
Df Residuals:                    1390   BIC:                         1.310e+04
Df Model:                           3
Covariance Type:            nonrobust
===================================================================================
                      coef    std err          t      P>|t|      [0.025      0.975]
```

```
-----------------------------------------------------------------------------------
Intercept          98.0027      5.324     18.408      0.000      87.559     108.446
SEX[T.male]        -6.0457      9.219     -0.656      0.512     -24.130      12.038
FRW                 0.4979      0.048     10.288      0.000       0.403       0.593
FRW:SEX[T.male]     0.0103      0.087      0.118      0.906      -0.161       0.182
==============================================================================
Omnibus:                      331.026   Durbin-Watson:                   1.768
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              852.312
Skew:                           1.250   Prob(JB):                    8.37e-186
Kurtosis:                       5.903   Cond. No.                     1.66e+03
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 1.66e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
```

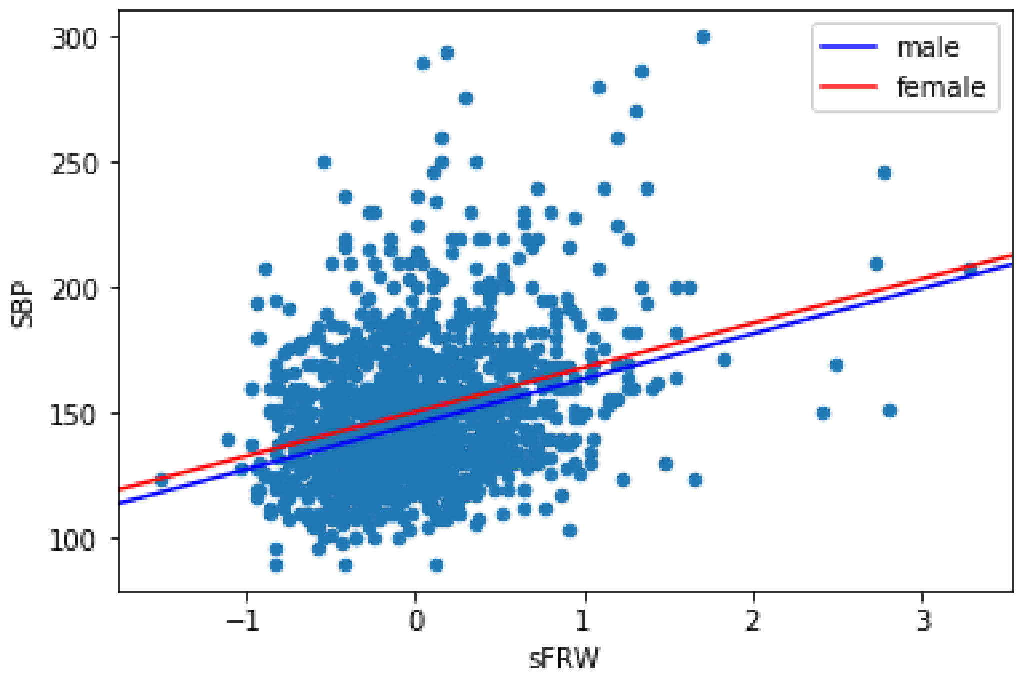
```
In [11]: # Renormalize to ease interpretation of the model parameters
         fram["sAGE"] = rescale(fram.AGE)
         fram["sFRW"] = rescale(fram.FRW)
         fram["sCHOL"] = rescale(fram.CHOL)
         fram["sCIG"] = rescale(fram.CIG)
         # Note: No need to scale the variable SEX
```

```
In [12]: # Now with renormalized variables
         fit3=smf.ols('SBP ~ sFRW + SEX + sFRW:SEX', data=fram).fit()
         print(fit3.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.118
Model:                            OLS   Adj. R-squared:                  0.116
Method:                 Least Squares   F-statistic:                     61.92
Date:                Thu, 25 Apr 2019   Prob (F-statistic):           1.42e-37
Time:                        22:08:32   Log-Likelihood:                -6536.3
No. Observations:                1394   AIC:                         1.308e+04
Df Residuals:                    1390   BIC:                         1.310e+04
Df Model:                           3
Covariance Type:            nonrobust
====================================================================================
                       coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------------
Intercept          150.4587      0.984    152.940      0.000     148.529     152.389
SEX[T.male]         -4.9569      1.437     -3.449      0.001      -7.776      -2.138
sFRW                17.6762      1.718     10.288      0.000      14.306      21.047
sFRW:SEX[T.male]     0.3669      3.106      0.118      0.906      -5.727       6.461
==============================================================================
Omnibus:                      331.026   Durbin-Watson:                   1.768
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              852.312
Skew:                           1.250   Prob(JB):                    8.37e-186
Kurtosis:                       5.903   Cond. No.                         5.27
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

```
In [13]: p=fit3.params
         fram.plot.scatter("sFRW", "SBP")
         #abline(p.Intercept + p["SEX[T.male]"],
         #       p.sFRW + p["sFRW:SEX[T.male]"], col="blue", label="male")
         #abline(p.Intercept, p.sFRW, col="red", label="female")
         int1 = p.Intercept + p["SEX[T.male]"]
         int2 = p.Intercept
         slope1 = p.sFRW + p["sFRW:SEX[T.male]"]
         slope2 = p.sFRW
         abline_plot(intercept=int1, slope=slope1, ax=plt.gca(), color="blue", label="male")
         abline_plot(intercept=int2, slope=slope2, ax=plt.gca(), color="red", label="female")
         plt.legend();
```



2.1 Background variables

ID	Explanation
SEX	Gender
AGE	Age at the start of the study
FRW	Weight in relation to groups median
SBP	Systolic Blood Pressure
DBP	Diastolic Blood Pressure
CHOL	Cholestherol level
CIG	Smoking (cigarets per day)

Next we add a continuous background variable: cholesterol.

```
In [14]: fit4=smf.ols('SBP ~ sFRW + SEX + sFRW:SEX + sCHOL', data=fram).fit()
         print(fit4.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.125
Model:                            OLS   Adj. R-squared:                  0.123
Method:                 Least Squares   F-statistic:                     49.75
Date:                Thu, 25 Apr 2019   Prob (F-statistic):           3.67e-39
Time:                        22:08:32   Log-Likelihood:                -6530.4
No. Observations:                1394   AIC:                         1.307e+04
Df Residuals:                    1389   BIC:                         1.310e+04
Df Model:                           4
Covariance Type:            nonrobust
=====================================================================================
                        coef    std err          t      P>|t|      [0.025      0.975]
-------------------------------------------------------------------------------------
Intercept         150.0166      0.988    151.776      0.000     148.078     151.955
SEX[T.male]        -4.0700      1.455     -2.798      0.005      -6.923      -1.216
sFRW               17.7594      1.712     10.375      0.000      14.402      21.117
sFRW:SEX[T.male]   -0.1272      3.098     -0.041      0.967      -6.204       5.950
sCHOL               4.9197      1.433      3.433      0.001       2.108       7.731
==============================================================================
Omnibus:                      327.586   Durbin-Watson:                   1.774
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              843.566
Skew:                           1.237   Prob(JB):                    6.64e-184
Kurtosis:                       5.899   Cond. No.                         5.28
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

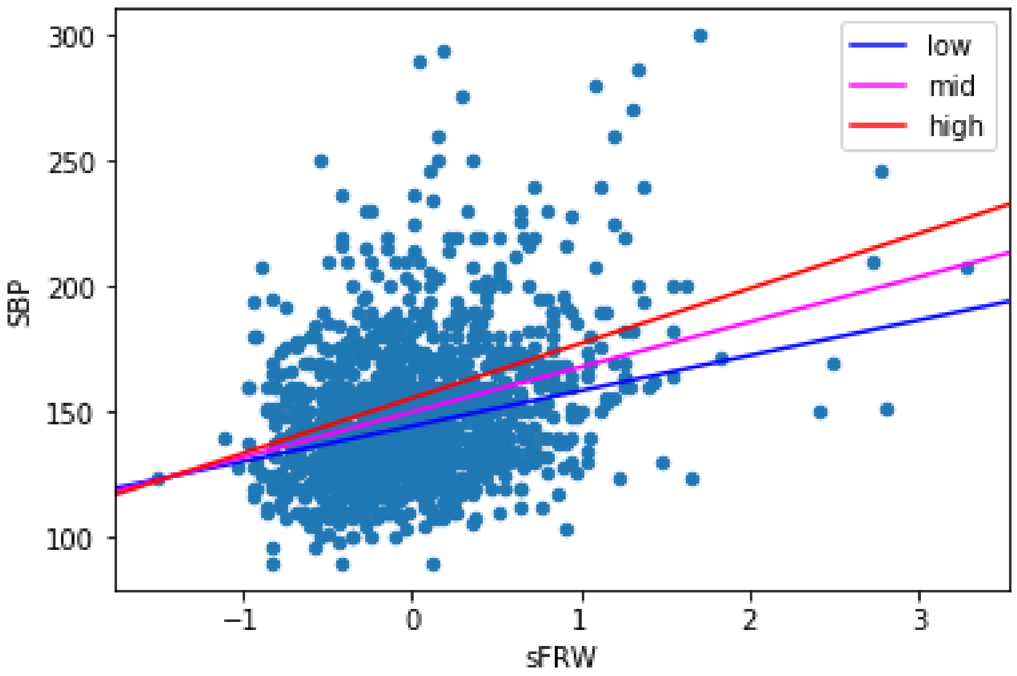
```
In [15]: # Add interactions between variables
         fit4=smf.ols('SBP ~ sFRW + SEX + sFRW:SEX + sCHOL + sCHOL:sFRW + sCHOL:SEX',
                      data=fram).fit()
         print(fit4.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                    SBP   R-squared:                       0.127
Model:                            OLS   Adj. R-squared:                  0.123
Method:                 Least Squares   F-statistic:                     33.58
Date:                Thu, 25 Apr 2019   Prob (F-statistic):           5.65e-38
Time:                        22:08:32   Log-Likelihood:                -6529.2
No. Observations:                1394   AIC:                         1.307e+04
Df Residuals:                    1387   BIC:                         1.311e+04
Df Model:                           6
Covariance Type:            nonrobust
=====================================================================================
                        coef    std err          t      P>|t|      [0.025      0.975]
-------------------------------------------------------------------------------------
Intercept           149.9420      0.994    150.850      0.000     147.992     151.892
SEX[T.male]          -4.0980      1.455     -2.816      0.005      -6.953      -1.243
sFRW                 17.9750      1.718     10.466      0.000      14.606      21.344
sFRW:SEX[T.male]      0.2760      3.108      0.089      0.929      -5.821       6.373
sCHOL                 5.5034      1.861      2.958      0.003       1.853       9.154
sCHOL:SEX[T.male]    -1.3225      2.939     -0.450      0.653      -7.087       4.442
sCHOL:sFRW            3.9052      2.741      1.425      0.154      -1.471       9.282
==============================================================================
Omnibus:                      318.099   Durbin-Watson:                   1.769
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              798.422
Skew:                           1.212   Prob(JB):                    4.22e-174
Kurtosis:                       5.805   Cond. No.                         5.32
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

Normalized data (rescale) allows analysis of the importance of variables. An interpretation: how much does a change of 2*standard deviation affect the explained variable. In the following we visualize women with either low, medium or high cholestherol.

```
In [16]: p=fit4.params
         fram.plot.scatter("sFRW", "SBP")
         abline_plot(intercept=p.Intercept - p["sCHOL"], slope=p.sFRW - p["sCHOL:sFRW"],
                     ax=plt.gca(), color="blue", label="low")
         abline_plot(intercept=p.Intercept, slope=p.sFRW,
                     ax=plt.gca(), color="magenta", label="mid")
         abline_plot(intercept=p.Intercept + p["sCHOL"], slope=p.sFRW + p["sCHOL:sFRW"],
                     ax=plt.gca(), color="red", label="high")
         plt.legend();
```



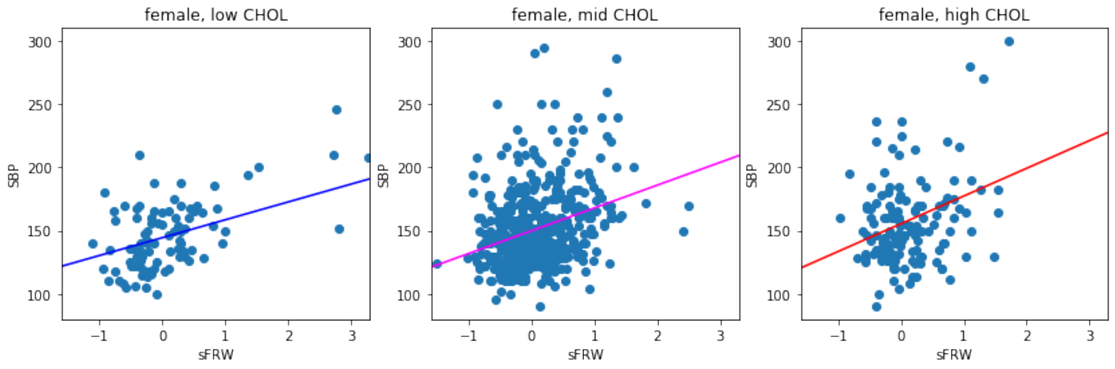
Below is the same analysis but in separate visualizations.

```
In [17]: fig, ax = plt.subplots(1,3, subplot_kw={"xlim": (-1.6, 3.3), "ylim": (80,310),
                                                  "xlabel": "sFRW", "ylabel": "SBP"},
                                figsize=(14, 4))
         ax[0].scatter(fram.sFRW[(fram.SEX=="female") & (fram.sCHOL < -0.5)],
                       fram.SBP[(fram.SEX=="female") & (fram.sCHOL < -0.5)])
         abline_plot(p.Intercept - p["sCHOL"],
                p.sFRW - p["sCHOL:sFRW"], color="blue", label="low", ax=ax[0])
         ax[0].set_title("female, low CHOL")

         ax[1].scatter(fram.sFRW[(fram.SEX=="female") & (fram.sCHOL > -0.5) &
                                 (fram.sCHOL < 0.5)],
                       fram.SBP[(fram.SEX=="female") & (fram.sCHOL > -0.5) &
                                (fram.sCHOL < 0.5)])
         abline_plot(p.Intercept, p.sFRW, color="magenta", label="mid", ax=ax[1])
         ax[1].set_title("female, mid CHOL")

         ax[2].scatter(fram.sFRW[(fram.SEX=="female") & (fram.sCHOL > 0.5)],
                       fram.SBP[(fram.SEX=="female") & (fram.sCHOL  > 0.5)])
         abline_plot(p.Intercept + p["sCHOL"],
                p.sFRW + p["sCHOL:sFRW"], color="red", label="high", ax=ax[2])
         ax[2].set_title("female, high CHOL")

Out[17]: Text(0.5, 1.0, 'female, high CHOL')
```



2.1.1 Prediction and generalization

Model's predictive accuracy in the data it was learned from does not give a good picture of its predictive capabilities: the model can be overfitted. A better estimate for the predictive accuracy can be obtained using cross validation: 1. Divide the data into parts for fitting and for validation 2. The model is fitted in a part of the data (training data) 3. The models is tested on another part of the data (test data). Then prediction error is computed. 4. This is repeated for a wanted number of divisions of the data

One model:

```
In [19]: train, test = train_test_split(fram)               # Split the date into two parts
         fit = smf.ols('SBP ~ sFRW + SEX + sCHOL', data=train).fit()  # Fit the model
         pred = fit.predict(test)                           # Compute predictions
         rmse = np.sqrt(np.mean((pred - test.SBP)**2))      # Root mean square error
         rmse
```

```
Out[19]: 27.234790574539684
```

Another model:

```
In [20]: train, test = train_test_split(fram)
         fit = smf.ols('SBP ~ sFRW + SEX + sCHOL + sFRW:SEX +  sCHOL:sFRW + sCHOL:SEX',
                       data=train).fit()
         pred = fit.predict(test)
         rmse = np.sqrt(np.mean((pred - test.SBP)**2))
         rmse
```

```
Out[20]: 26.560076340037707
```

Let's repeat this random data splitting 100 times for both models and compute the average RMSEs:

```
In [21]: error_basic=[]
         error_interact=[]
         np.random.seed(9)
```

```
        for i in range(100):
            train, test = train_test_split(fram)
            fit1 = smf.ols('SBP ~ sFRW + SEX + sCHOL', data=train).fit()
            fit2 = smf.ols('SBP ~ sFRW + SEX + sCHOL + sFRW:SEX +  sCHOL:sFRW + sCHOL:SEX',
                           data=train).fit()
            pred1 = fit1.predict(test)
            pred2 = fit2.predict(test)
            error_basic.append(np.sqrt(np.mean((pred1 - test.SBP)**2)))
            error_interact.append(np.sqrt(np.mean((pred2 - test.SBP)**2)))
        pd.Series(error_basic).mean(), pd.Series(error_interact).mean()
```

```
Out[21]: (26.18486951586637, 26.259898342406064)
```

We can use the *Mann–Whitney U test* to see whether the prediction errors differ significantly.

```
In [22]: statsmodels.stats.stattools.stats.mannwhitneyu(error_basic, error_interact,
                                                       alternative="two-sided")
```

```
Out[22]: MannwhitneyuResult(statistic=4857.0, pvalue=0.7277028167772348)
```

Let's change the first model and redo the experiment:

```
In [23]: error_basic=[]
         error_interact=[]
         np.random.seed(9)
         for i in range(100):
             train, test = train_test_split(fram)
             fit1 = smf.ols('SBP ~ sFRW ', data=train).fit()
             fit2 = smf.ols('SBP ~ sFRW + SEX + sCHOL + sFRW:SEX +  sCHOL:sFRW + sCHOL:SEX',
                            data=train).fit()
             pred1 = fit1.predict(test)
             pred2 = fit2.predict(test)
             error_basic.append(np.sqrt(np.mean((pred1 - test.SBP)**2)))
             error_interact.append(np.sqrt(np.mean((pred2 - test.SBP)**2)))
         pd.Series(error_basic).mean(), pd.Series(error_interact).mean()
```

```
Out[23]: (26.38389912270515, 26.259898342406064)
```

```
In [24]: statsmodels.stats.stattools.stats.mannwhitneyu(error_basic, error_interact,
                                                       alternative="two-sided")
```

```
Out[24]: MannwhitneyuResult(statistic=5222.0, pvalue=0.5883624055865182)
```

Now let's change the second model:

```
In [25]: error_basic=[]
         error_interact=[]
         np.random.seed(9)
         for i in range(100):
             train, test = train_test_split(fram)
```

```
            fit1 = smf.ols('SBP ~ sFRW ', data=train).fit()
            fit2 = smf.ols('SBP ~ sFRW + SEX + sCHOL + sAGE + sCIG', data=train).fit()
            pred1 = fit1.predict(test)
            pred2 = fit2.predict(test)
            error_basic.append(np.sqrt(np.mean((pred1 - test.SBP)**2)))
            error_interact.append(np.sqrt(np.mean((pred2 - test.SBP)**2)))
        pd.Series(error_basic).mean(), pd.Series(error_interact).mean()
```

```
Out[25]: (26.38389912270515, 25.924525100203073)
```

```
In [26]: statsmodels.stats.stattools.stats.mannwhitneyu(error_basic, error_interact,
                                                        alternative="two-sided")
```

```
Out[26]: MannwhitneyuResult(statistic=5742.0, pvalue=0.0700213003206784)
```

3 Logistic regression

Topics:

- Logistic regression model
- Classification problems

Learning targets:

- Fit logistic regression models with Python
- Interpret the estimated regression models

3.1 Regression model is transformations of variables

Multi-variable linear regression model:

$$y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$$

The model is very flexible with respect to the variables x_{ij} and y_i: the variables need not be direct observations, for example the interaction terms like `SEX:sWHP`. Also transformations of variables are permitted, for example `SBP ~ log(FRW) + sFRW + SEX + SEX:sFRW`.

For example, logarithm transform is often useful for variables, whose range is large and whose effect can be expected to saturate. An example: `log(SBP) ~ log(FRW) + SEX + SEX:log(FRW)`

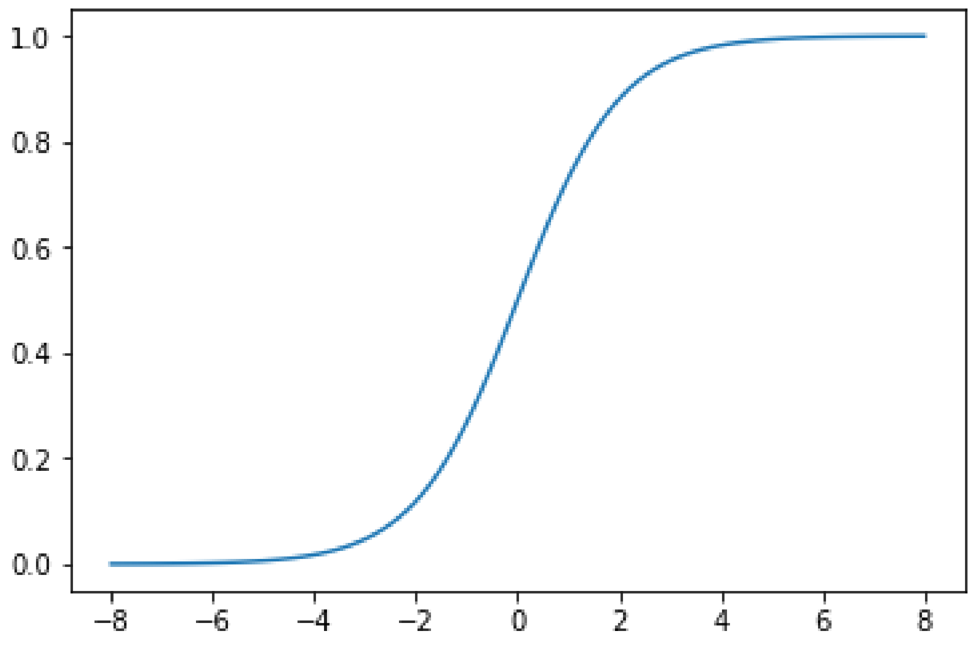
$$SBP = \alpha FRW^{\beta_1} \exp(SEX)^{\beta_2} FRW^{SEX \cdot \beta_3}$$

3.2 Binary target variable (classification)

It is not sensible to try to predict a binary variable directly using linear regression. In general, we want to predict $p(y_i = \text{TRUE} \mid X)$. In linear regression the possible values are in the interval $(-\infty, \infty)$, whereas probabilities are in the interval $[0, 1]$. The idea is to transform the unrestricted predictions to probabilities.

```
In [27]: def logistic(x):
             return 1.0 / (1.0 + np.exp(-x))
```

```
In [28]: X=np.linspace(-8, 8, 100)
         plt.plot(X, logistic(X));
```



$$\mathrm{logit}^{-1}(x) = \frac{1}{1+\exp(-x)}$$

Logistic transform is non-linear: same change in input produces different changes in probabilities. The speed of change is at its largest at the point $x = 0 : f'(0) = 1/4$. Logistic regression is the most common tool for classification. It can also be used to recognize variables that are important to the classification.

Let's continue with the fram data. First we define a diagnose for high blood pressure.

```
In [29]: fram["HIGH_BP"] = (fram.SBP >= 140) | (fram.DBP >= 90)
         fram.HIGH_BP.head()

Out[29]: 0    True
         1    True
         2    True
         3    True
         4    True
         Name: HIGH_BP, dtype: bool

In [30]: fram.HIGH_BP.value_counts()

Out[30]: True     906
         False    488
         Name: HIGH_BP, dtype: int64
```

```
In [31]: fram.HIGH_BP = fram.HIGH_BP.map(int)
```

Note that for boolean variables we use type `int` here instead of `bool`, because we want to make the encoding of booleans as integers explicit: `0` for `False` and `1` for `True`. (The implicit encoding of booleans as integers in statsmodels library is unfortunately inconsistent.)

```
In [32]: fram.HIGH_BP.mean()        # Fraction of observations with this diagnose

Out[32]: 0.6499282639885222

In [33]: fram.head()

Out[33]:      ID     SEX  AGE  FRW  SBP  SBP10  DBP  CHOL  CIG  CHD YRS_CHD  DEATH  \
         0  4988  female   57  135  186    NaN  120   150    0    1     pre      7
         1  3001  female   60  123  165    NaN  100   167   25    0      16     10
         2  5079  female   54  115  140    NaN   90   213    5    0       8      8
         3  5162  female   52  102  170    NaN  104   280   15    0      10      7
         4  4672  female   45   99  185    NaN  105   326   20    0       8     10

            YRS_DTH    CAUSE      sAGE      sFRW     sCHOL      sCIG  HIGH_BP
         0       11  unknown  0.477764  0.834668 -0.914016 -0.346569        1
         1       17  unknown  0.791473  0.496687 -0.730446  0.732493        1
         2       13  unknown  0.164056  0.271367 -0.233727 -0.130757        1
         3       11  unknown -0.045083 -0.094779  0.489755  0.300868        1
         4       17  unknown -0.777070 -0.179274  0.986475  0.516680        1
```

Let's fit a logistic regression model:

```
In [34]: fit1 = smf.glm(formula="HIGH_BP ~ FRW", data=fram,
                        family=sm.families.Binomial(statsmodels.genmod.families.links.logit)).
         fit1.summary()

Out[34]: <class 'statsmodels.iolib.summary.Summary'>
         """
                          Generalized Linear Model Regression Results
         ==============================================================================
         Dep. Variable:                HIGH_BP   No. Observations:                 1394
         Model:                            GLM   Df Residuals:                     1392
         Model Family:                Binomial   Df Model:                            1
         Link Function:                  logit   Scale:                          1.0000
         Method:                          IRLS   Log-Likelihood:                -858.64
         Date:                Thu, 25 Apr 2019   Deviance:                       1717.3
         Time:                        22:08:40   Pearson chi2:                 1.39e+03
         No. Iterations:                     4   Covariance Type:             nonrobust
         ==============================================================================
                          coef    std err          z      P>|z|      [0.025      0.975]
         ------------------------------------------------------------------------------
         Intercept     -2.8912      0.404     -7.158      0.000      -3.683      -2.100
         FRW            0.0339      0.004      8.650      0.000       0.026       0.042
         ==============================================================================
         """
```

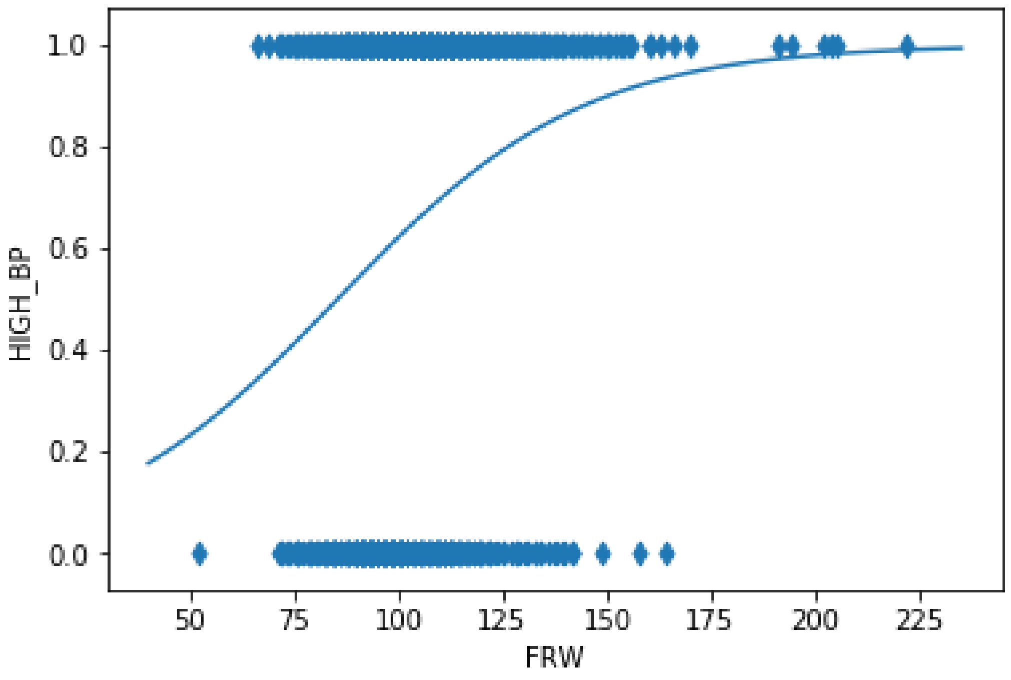
```
In [35]: fit1.params
```

```
Out[35]: Intercept   -2.891166
         FRW          0.033852
         dtype: float64
```

The R^2 is not sensible now. Instead, we use *deviance*, which measures the error. Smaller value is better. The coefficients are mostly like in linear regression. Also, the significance interpretation is the same. Coefficient β: change of one unit in a variable causes a change in the probability which is at most $\beta/4$.

```
In [36]: # Visualization of the model
         plt.scatter(fram.FRW, fram.HIGH_BP, marker="d")
         X=np.linspace(40, 235, 100)
         plt.plot(X, logistic(X*fit1.params.FRW + fit1.params.Intercept))
         plt.xlabel("FRW")
         plt.ylabel("HIGH_BP")
```

```
Out[36]: Text(0, 0.5, 'HIGH_BP')
```

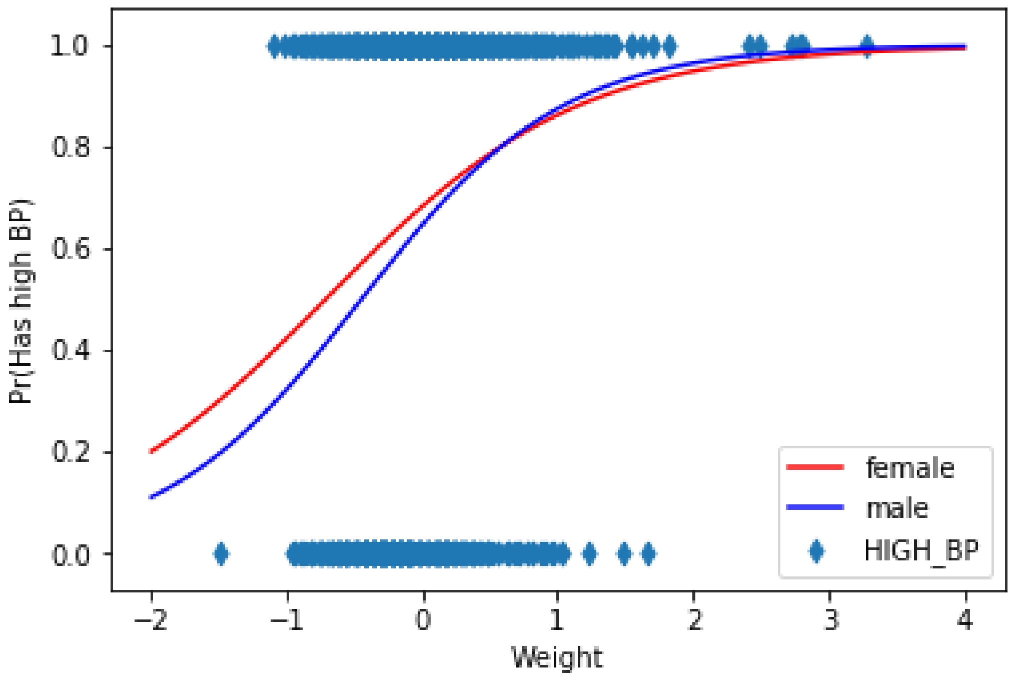


Next we add the gender and its interaction to the model:

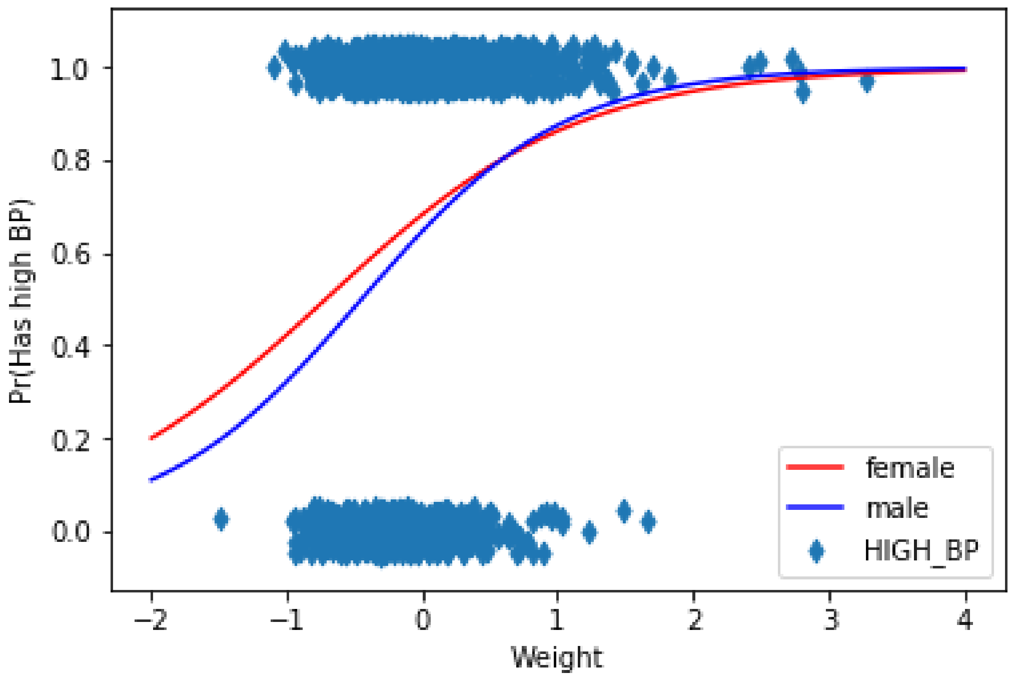
```
In [37]: fit2 = smf.glm(formula="HIGH_BP ~ sFRW + SEX + SEX:sFRW", data=fram,
                        family=sm.families.Binomial()).fit()
         fit2.summary()
```

```
Out[37]: <class 'statsmodels.iolib.summary.Summary'>
         """
                          Generalized Linear Model Regression Results
         ==============================================================================
         Dep. Variable:                HIGH_BP   No. Observations:                 1394
         Model:                            GLM   Df Residuals:                     1390
         Model Family:                Binomial   Df Model:                            3
         Link Function:                  logit   Scale:                          1.0000
         Method:                          IRLS   Log-Likelihood:                -856.87
         Date:                Thu, 25 Apr 2019   Deviance:                       1713.7
         Time:                        22:08:40   Pearson chi2:                 1.39e+03
         No. Iterations:                     4   Covariance Type:             nonrobust
         ====================================================================================
                                coef    std err          z      P>|z|      [0.025      0.975]
         ------------------------------------------------------------------------------------
         Intercept            0.7631      0.082      9.266      0.000       0.602       0.925
         SEX[T.male]         -0.1624      0.120     -1.350      0.177      -0.398       0.073
         sFRW                 1.0738      0.176      6.095      0.000       0.728       1.419
         SEX[T.male]:sFRW     0.2709      0.287      0.943      0.346      -0.292       0.834
         ====================================================================================
         """
```

```
In [38]: plt.scatter(fram.sFRW, fram.HIGH_BP, marker="d")
         X=np.linspace(-2, 4, 100)
         p = fit2.params
         plt.plot(X, logistic(X*p.sFRW + p.Intercept), color="red", label="female")
         plt.plot(X, logistic(X*(p.sFRW + p["SEX[T.male]:sFRW"]) +
                              p["SEX[T.male]"] + p.Intercept), color="blue", label="male")
         plt.xlabel("Weight")
         plt.ylabel("Pr(Has high BP)")
         plt.legend();
```



```
In [39]: # We add a bit of random jitter to the y value
         plt.scatter(fram.sFRW, fram.HIGH_BP + np.random.uniform(-0.05, 0.05, len(fram)),
                     marker="d")
         X=np.linspace(-2, 4, 100)
         p = fit2.params
         plt.plot(X, logistic(X*p.sFRW + p.Intercept), color="red", label="female")
         plt.plot(X, logistic(X*(p.sFRW + p["SEX[T.male]:sFRW"]) +
                          p["SEX[T.male]"] + p.Intercept), color="blue", label="male")
         plt.xlabel("Weight")
         plt.ylabel("Pr(Has high BP)")
         plt.legend();
```



3.3 Prediction

The `fittedvalues` attribute contains the predicted probabilities for each data point. Let's compute the fraction of mispredictions:

```
In [40]: error_rate = np.mean(((fit2.fittedvalues < 0.5) & fram.HIGH_BP) |
                              ((fit2.fittedvalues > 0.5) & ~fram.HIGH_BP))
         error_rate
```

```
Out[40]: 0.35581061692969873
```

What is a good error rate? For a random guess (tossing a coin): error rate is 50%. If we always choose the most common option, the error rate is less that 50%, sometimes a lot less.

```
In [41]: print("Base rate:", 1-np.mean(fram.HIGH_BP))
```

```
Base rate: 0.3500717360114778
```

3.4 Cross validation

```
In [42]: train, test = train_test_split(fram, seed=0)
         print(len(train), len(test))
         fit = smf.glm(formula="HIGH_BP ~ sFRW + SEX + SEX:sFRW", data=train,
                         family=sm.families.Binomial(statsmodels.genmod.families.links.logit))
```

```
        print(fit.summary())
        #print(test.head())
        pred = fit.predict(test, transform=True)
        #print(pred.describe())
        #print("Min:", pred.min())
        #print("Max:", pred.max())
        error_rate = np.mean(((pred < 0.5) & (test.HIGH_BP==1)) |
                             ((pred > 0.5) & (test.HIGH_BP==0)))
        print(error_rate, 1 - test.HIGH_BP.mean())
```

```
1115 279
                 Generalized Linear Model Regression Results
==============================================================================
Dep. Variable:                HIGH_BP   No. Observations:                 1115
Model:                            GLM   Df Residuals:                     1111
Model Family:                Binomial   Df Model:                            3
Link Function:                  logit   Scale:                          1.0000
Method:                          IRLS   Log-Likelihood:                -689.76
Date:                Thu, 25 Apr 2019   Deviance:                       1379.5
Time:                        22:08:41   Pearson chi2:                 1.11e+03
No. Iterations:                     4   Covariance Type:             nonrobust
====================================================================================
                       coef    std err          z      P>|z|      [0.025      0.975]
------------------------------------------------------------------------------------
Intercept            0.8008      0.092      8.752      0.000       0.621       0.980
SEX[T.male]         -0.2329      0.134     -1.743      0.081      -0.495       0.029
sFRW                 0.9641      0.197      4.895      0.000       0.578       1.350
SEX[T.male]:sFRW     0.1760      0.315      0.558      0.577      -0.442       0.794
====================================================================================
0.35125448028673834 0.36200716845878134
```

```
In [43]: error_model=[]
         error_null=[]
         np.random.seed(1)
         for i in range(100):
             train, test = train_test_split(fram)
             fit = smf.glm(formula="HIGH_BP ~ sFRW + SEX + SEX:sFRW", data=train,
                           family=sm.families.Binomial(statsmodels.genmod.families.links.logi
             #print(model.summary())
             pred = fit.predict(test, transform=True)
             error_rate = np.mean(((pred < 0.5) & (test.HIGH_BP==1)) |
                                  ((pred > 0.5) & (test.HIGH_BP==0)))
             error_model.append(error_rate)
             error_null.append((1 - test.HIGH_BP).mean())
         #for model, null in zip(error_model, error_null):
         #    print(model, null)
         pd.Series(error_model).mean(), pd.Series(error_null).mean()
```

```
Out[43]: (0.3520071684587814, 0.3488530465949821)
```

Test to see whether the results are significantly different:

```
In [44]: statsmodels.stats.stattools.stats.mannwhitneyu(error_model, error_null,
                                                        alternative="two-sided")
```

```
Out[44]: MannwhitneyuResult(statistic=5312.5, pvalue=0.44539961439180353)
```

Let's define another diagnose:

```
In [45]: fram["HIGH_BP2"] = (fram.SBP > 140) | (fram.DBP > 90)
         fram["HIGH_BP2"] = fram["HIGH_BP2"].map(int)
         fram["HIGH_BP2"].mean()
```

```
Out[45]: 0.56025824964132
```

```
In [46]: error_model=[]
         error_null=[]
         np.random.seed(9)
         for i in range(100):
             train, test = train_test_split(fram)
             fit = smf.glm(formula="HIGH_BP2 ~ sFRW + SEX + SEX:sFRW", data=train,
                                 family=sm.families.Binomial()).fit()
             #print(model.summary())
             pred = fit.predict(test)
             error_rate = np.mean(((pred < 0.5) & (test.HIGH_BP2==1)) |
                                     ((pred > 0.5) & (test.HIGH_BP2==0)))
             error_model.append(error_rate)
             error_null.append((1-test.HIGH_BP2).mean())
         #for model, null in zip(error_model, error_null):
         #    print(model, null)
         pd.Series(error_model).mean(), pd.Series(error_null).mean()
```

```
Out[46]: (0.3860931899641578, 0.4403942652329749)
```

Test again:

```
In [47]: statsmodels.stats.stattools.stats.mannwhitneyu(error_model, error_null,
                                                        alternative="two-sided")
```

```
Out[47]: MannwhitneyuResult(statistic=525.0, pvalue=7.3782255350127615e-28)
```