nhanes_ols

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1 Basic regression using Python and Statsmodels – a case study using the NHANES data

This notebook introduces some of the main ideas of regression analysis, focusing on the practical aspects of fitting regression models in Python using the Statsmodels package. We will also be using the Pandas library for data management, and the Numpy library for numerical calculations.

At a high level, regression analysis is a way of relating *inputs* to *outputs*. For example, if we want to understand how the fuel efficiency of a car, measured in gallons per mile, relates to the vehicle's weight and engine displacement, then vehicle weight and engine displacement could be taken as the inputs, with fuel efficiency as the output. Note that this does not mean that we view vehicle weight and engine displacement as being the only direct determinants of fuel efficiency. For example, the cross sectional area of the vehicle would also matter a lot (for aerodynamics). Regression modeling can be used when we have one or more input factors that may partially explain the output, allowing us to estimate how the inputs and outputs are statistically related.

Regression analysis has a long history, with roots in many different fields. As a result, there are multiple terms for many of the key concepts. For example, the "output" discussed above is often called the *dependent variable*, the *outcome*, or the *response*. The "inputs" discussed above are often called the *covariates*, *regressors*, or *independent variables*.

2 Regression analysis and conditional distributions

A more formal way of looking at regression analysis is through the idea of a *conditional distribution*. Switching to another example let y denote a person's blood pressure, and let a and g denote their age and gender, respectively. Our data represent a population, for example, all adults in the United States. There is a "marginal mean" of all blood pressure values in this population, which can be estimated using the sample mean (average value) of all the blood pressure values in our data set. There are also many different "conditional means", which capture the mean blood pressure for the subset of all adults in the US having a particular age and gender.

It is common to use the term "expectation" to refer to a mean or average value in a population, and denote it by the letter "E". Thus, $E[y]$ is the (marginal) expected blood pressure for all US adults, and $E[y \mid a, g]$ is the conditional mean blood pressure for all adults of a particular age and gender. For example, $E[y \mid a = 35, g = F]$ is the conditional mean blood pressure for all 35 year-old women in our population.

Directly analogous to conditional means is the concept of "conditional variance". The marginal variance $Var[y]$ is the variance (expected squared deviation from the mean) of the whole population. The conditional variance $Var[y \mid a = 35, g = F]$ is the variance of y for the subpopulation of 35 year-old women.

As with most forms of statistical analysis, the goal of regression is to use the sample to learn about the population, and to quantify the uncertainty in doing so. Since we have a finite sample of data, we are not able to recover $E[y \mid a, g]$ directly, but rather will only be able to estimate it. We can then use the tools of statistical inference (e.g. standard errors, confidence intervals, and hypothesis tests) to assess how precisely we have recovered the "estimation target" $E[y \mid a, g]$.

3 NHANES

The National Health and Nutrition Examination Study (NHANES) is a study sponsored by the US government that has run in waves since the 1970's. Each NHANES wave is a cross sectional study of around 10,000 people, selected to represent the US adult population at a particular point in time. A large number of measures are made on each of the NHANES subjects. Here we will focus on basic demographic characteristics, body dimensions (e.g. height or BMI), and blood pressure (systolic and diastolic, measured three times each).

Note that the NHANES data were collected as a designed survey, and in general should be analyzed as such. This means that survey design information such as sampling weights, strata, and clusters should be accounted for in any analysis using NHANES. But to introduce how linear regression is most commonly used, we will not incorporate the survey structure of the NHANES sample into the analyses conducted here.

We begin by importing the libraries that we will be using.

[1]:

```
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
import statsmodels.api as sm
import numpy as np
```

```
/nfs/kshedden/python3/lib/python3.7/site-
packages/statsmodels/compat/pandas.py:23: FutureWarning: The Panel class is
removed from pandas. Accessing it from the top-level namespace will also be
removed in the next version
  data_klasses = (pandas.Series, pandas.DataFrame, pandas.Panel)
```

Next we will load the data. The NHANES study encompasses multiple waves of data collection. Here we will only use the 2015-2016 data. As with most data sets, there are some missing values in the NHANES files. While many of the methods demonstrated below would handle missing values automatically (at least in a crude way), here we drop up-front all rows with missing values in any of the key variables that we will use in this notebook.

[2]:

```
url = "https://raw.githubusercontent.com/kshedden/statswpy/master/NHANES/merged/
  ↪nhanes_2015_2016.csv"
da = pd.read_csv(url)
```

[3]:

```
# Drop unused columns, drop rows with any missing values.
vars = ["BPXSY1", "RIDAGEYR", "RIAGENDR", "RIDRETH1", "DMDEDUC2", "BMXBMI",␣
  ↪"SMQ020"]
da = da[vars].dropna()
```

4 Linear regression and least squares

The *regression function* $E[y|x]$ (for one or more covariates x) could in principle be any function of x, i.e. a mathematical function mapping vectors x to real numbers y. To make the analysis more tractable, many forms of regression analysis estimate $E[y|x]$ by modeling it, often in a parametric form. Specifically, we may use the *linear mean structure*

$$E[y|x] = b_0 + b_1x_1 + \cdots + b_px_p.$$

This mean structure implies that when comparing two observations whose values of a covariate, say x_j, differ by one unit, and that are identical in terms of all other covarates, then the expected values of the dependent variable for these two observations will differ by b_j units.

Note that using a linear mean structure does not imply that we are limited to modeling linear phenomena. The covariates x_j can themselves be nonlinear functions of other covariates, allowing us to capture many nonlinear relationships using linear regression. We will discuss this point in more detail below.

The most widely-used approach for fitting models with linear mean structures to observed data sets is *least squares*. We will not discuss the theory of least squares analysis here further, except to note that it has a number of good properties, including being fast to compute, and allowing for relatively straightforward statistical inference. Although there are some settings where least squares is known to perform poorly, in many commonly-encountered settings it should give meaningful results and be competitive in performance with any other approach.

5 Regression analysis with the NHANES data

We will focus initially on regression models in which systolic blood pressure (SBP) is the outcome (dependent) variable. That is, we will predict SBP from other variables. SBP is an important indicator of cardiovascular health. It tends to increase with age, is greater for overweight people (i.e. people with greater body mass index or BMI), and also differs among demographic groups, for example among gender and ethnic groups.

Since SBP is a quantitative variable, we will model it using least squares to fit a regression model with a linear mean structure. This is commonly referred to as simply "linear regression". While linear regression is commonly used with quantitative outcome variables, it is not the only regression method that can be used with quantitative outcomes, nor is it the case that linear regression can only be used with quantitative outcomes. However, linear regression is a good default starting point for any regression analysis involving a quantitative outcome variable.

5.1 Interpreting regression parameters in a basic model

We start with a simple linear regression model with only one covariate, age, predicting SBP. In the NHANES data, the variable BPXSY1 contains the first recorded measurement of SBP for a subject, and RIDAGEYR is the subject's age in years. The model that is fit in the next code cell expresses the expected SBP as a linear function of age:

[4]:

```
model = sm.OLS.from_formula("BPXSY1 ~ RIDAGEYR", data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.207
Model:                            OLS   Adj. R-squared:                  0.207
Method:                 Least Squares   F-statistic:                     1333.
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          2.09e-259
Time:                        15:01:14   Log-Likelihood:                -21530.
No. Observations:                5102   AIC:                         4.306e+04
Df Residuals:                    5100   BIC:                         4.308e+04
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept    102.0935      0.685    149.120      0.000     100.751     103.436
RIDAGEYR       0.4759      0.013     36.504      0.000       0.450       0.501
==============================================================================
Omnibus:                      690.261   Durbin-Watson:                   2.039
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1505.999
Skew:                           0.810   Prob(JB):                         0.00
Kurtosis:                       5.112   Cond. No.                         156.
==============================================================================

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

Much of the output above is not relevant for us, so focus on the center section of the output where the header row begins with **coef**. This section contains the estimated values of the parameters of the regression model, their standard errors, and other values that are used to quantify the uncertainty in the regression parameter estimates. Note that the parameters of a regression model, which appear in the column labeled **coef** in the table above, may also be referred to as *slopes* or *effects*.

This fitted model implies that when comparing two people whose ages differ by one year, the older person will on average have 0.48 units higher SBP than the younger person. This difference is statistically significant, based on the p-value shown under the column labeled `P>|t|`. This means that there is strong evidence that there is a real association between between systolic blood pressure and age in this population.

SBP is measured in units of *millimeters of mercury*, expressed *mm/Hg*. In order to better understand the meaning of the estimated regression parameter 0.48, we can look at the standard deviation of SBP:

[5]:
```
da.BPXSY1.std()
```

[5]:
```
18.486559500781865
```

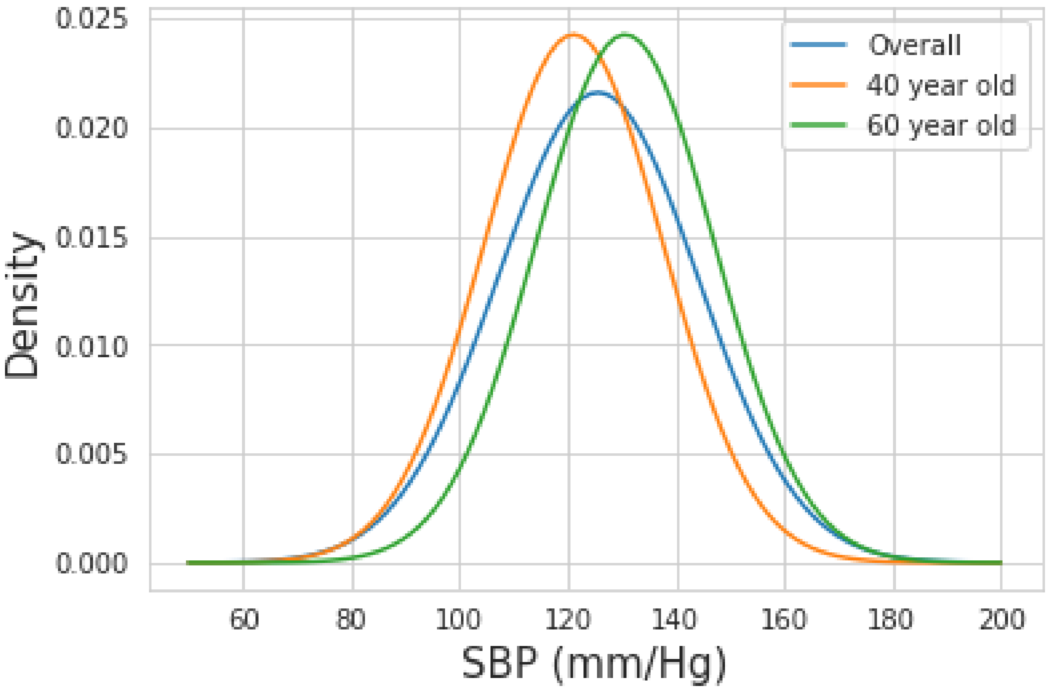
The standard deviation of around 18.5 tells us that a randomly selected person from the population has SBP that deviates by around 18.5 mm/Hg on average from the population mean SBP value. Thus, there are around 18.5 standard deviation units of variation in the outcome that we are studying here. The goal of a regression analysis is to explain this variation using other known factors.

The standard deviation of around 18.5 is large compared to the regression slope of 0.48. However the regression slope corresponds to the change in average SBP for a single year of age, and this effect accumulates with age. Comparing a 40 year-old person to a 60 year-old person, there is a 20 year difference in age, which translates into a `20 * 0.48 = 9.6` unit difference in average SBP between these two people. This difference is around half of one standard deviation, and would generally be considered to be an important and meaningful shift.

Below we visualize the distributions of SBP for the whole population (i.e. the marginal distribution), and for the subpopulations of people who are 40 and 60 years old, respectively. This visualization is based on a model that has been fit to the data. It may be misleading if the model do not fit the data well. This is an important topic, but we will set it aside for now.

[6]:

```
sbp = np.linspace(50, 200, 100) # Grid of possible blood pressure values
mn0 = da.BPXSY1.mean() # marginal mean blood pressure
sd0 = da.BPXSY1.std() # marginal SD of blood pressure

from scipy.stats.distributions import norm

y0 = norm.pdf(sbp, mn0, sd0)

mn1 = np.dot(result.params, [1, 40]) # Conditional mean for a 40 year old␣
 ↪person
sd1 = np.sqrt(result.scale)
y1 = norm.pdf(sbp, mn1, sd1)

mn2 = np.dot(result.params, [1, 60]) # Conditional mean for a 60 year old␣
 ↪person
sd2 = np.sqrt(result.scale)
y2 = norm.pdf(sbp, mn2, sd2)

sns.set_style("whitegrid")
ax = sns.lineplot(sbp, y0, label="Overall")
sns.lineplot(sbp, y1, label="40 year old")
sns.lineplot(sbp, y2, label="60 year old")
ax.set_xlabel("SBP (mm/Hg)", size=15)
_ = ax.set_ylabel("Density", size=15)
```



5.2 R-squared and correlation

In the case of regression with a single independent variable, there is a very close correspondence between a linear regression analysis and a Pearson correlation analysis. The primary summary statistic for assessing the strength of a predictive relationship in a regression model is the *R-squared*, which is shown to be 0.207 in the regression output above. This means that 21% of the variation in SBP is explained by age. Note that this value is exactly the same as the squared Pearson correlation coefficient between SBP and age, as shown below.

[7]:
```
cc = da[["BPXSY1", "RIDAGEYR"]].corr()
print(cc.BPXSY1.RIDAGEYR**2)
```

```
0.20715459625188243
```

There is a second way to interpret the R-squared, which makes use of the *fitted values* of the regression. The fitted values are predictions of the blood pressure for each person in the data set, based on their covariate values. In this case, the only covariate is age, so we are predicting each NHANES subject's blood pressure as a function of their age. If we calculate the Pearson correlation coefficient between the fitted values from the regression, and the actual SBP values, and then square this correlation coefficient, we see that we again get the R-squared from the regression model:

[8]:
```
cc = np.corrcoef(da.BPXSY1, result.fittedvalues)
print(cc[0, 1]**2)
```

```
0.2071545962518695
```

Thus, we see that in a linear model fit with only one covariate, the regression R-squared is equal to the squared Pearson correlation between the covariate and the outcome, and is also equal to the squared Pearson correlation between the fitted values and the outcome.

5.3 Adding a second variable

Above we considered a simple linear regression analysis with only one covariate (age) predicting systolic blood pressure (SBP). The real power of regression analysis arises when we have more than one covariate predicting an outcome. As noted above, SBP is expected to be related to gender as well as to age, so we next add gender to the model. The NHANES variable for gender is named RIAGENDR.

We begin by creating a relabeled version of the gender variable:

[9]:
```
# Create a labeled version of the gender variable
da["RIAGENDRx"] = da.RIAGENDR.replace({1: "Male", 2: "Female"})
```

Now we are ready to fit the linear model:

[10]:
```
model = sm.OLS.from_formula("BPXSY1 ~ RIDAGEYR + RIAGENDRx", data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.215
Model:                            OLS   Adj. R-squared:                  0.214
Method:                 Least Squares   F-statistic:                     697.4
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          1.87e-268
Time:                        15:01:15   Log-Likelihood:                -21505.
No. Observations:                5102   AIC:                         4.302e+04
Df Residuals:                    5099   BIC:                         4.304e+04
Df Model:                           2
Covariance Type:            nonrobust
================================================================================
=====
                        coef    std err          t      P>|t|      [0.025
0.975]
--------------------------------------------------------------------------------
-----
Intercept            100.6305      0.712    141.257      0.000      99.234
102.027
RIAGENDRx[T.Male]      3.2322      0.459      7.040      0.000       2.332
4.132
RIDAGEYR               0.4739      0.013     36.518      0.000       0.448
0.499
==============================================================================
Omnibus:                      706.732   Durbin-Watson:                   2.036
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1582.730
Skew:                           0.818   Prob(JB):                         0.00
Kurtosis:                       5.184   Cond. No.                         168.
```

```
==============================================================================

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

The syntax `RIDAGEYR + RIAGENDRx` in the cell above does not mean that these two variables are literally added together. Instead, it means that these variables are both included in the model as predictors of blood pressure (`BPXSY1`).

The model that was fit above uses both age and gender to explain the variation in SBP. It finds that two people with the same gender whose ages differ by one year tend to have blood pressure values differing by 0.47 units, which is essentially the same role for age that we found above in the model based on age alone. This model also shows us that comparing a man and a woman of the same age, the man will on average have 3.23 units greater SBP.

It is very important to emphasize that the age coefficient of 0.47 is only meaningful when comparing two people of the same gender, and the gender coefficient of 3.23 is only meaningful when comparing two people of the same age. Moreover, these effects are additive, meaning that if we compare, say, a 50 year old man to a 40 year old woman, the man's blood pressure will on average be around 3.23 + 10*0.47 = 7.93 units higher, with the first term in this sum being attributable to gender, and the second term being attributable to age.

We noted above that the regression coefficient for age did not change by much when we added gender to the model. It is important to note however that in general, the estimated coefficient of a variable in a regression model will change when other variables are added or removed. We see here that a coefficient is nearly unchanged if any variables that are added to or removed from the model are approximately uncorrelated with the other covariates that are already in the model.

Below we confirm that gender and age are nearly uncorrelated in this data set (the correlation of around -0.02 is negligible):

[11]:
```python
# We need to use the original, numerical version of the gender
# variable to calculate the correlation coefficient.
da[["RIDAGEYR", "RIAGENDR"]].corr()
```

[11]:
```
          RIDAGEYR  RIAGENDR
RIDAGEYR  1.000000 -0.021398
RIAGENDR -0.021398  1.000000
```

Observe that in the regression output shown above, an R-squared value of 0.215 is listed. Earlier we saw that for a model with only one covariate, the R-squared from the regression could be defined in two different ways, either as the squared correlation coefficient between the covariate and the outcome, or as the squared correlation coefficient between the fitted values and the outcome. When more than one covariate is in the model, only the second of these two definitions continues to hold:

[12]:
```python
cc = np.corrcoef(da.BPXSY1, result.fittedvalues)
print(cc[0, 1]**2)
```

```
0.21478581086243798
```

5.4 Categorical variables and reference levels

In the model fit above, gender is a categorical variable, and only a coefficient for males is included in the regression output (i.e. there is no coefficient for females in the tables above). Whenever a categorical variable is used as a covariate in a regression model, one level of the variable is omitted and is automatically given a coefficient of zero. This level is called the *reference level* of the covariate. Here, the female level of the gender variable is the reference level. This does not mean that being a woman has no impact on blood pressure. It simply means that we have written the model so that female blood pressure is the default, and the coefficient for males (3.23) shifts the blood pressure away from the default.

We could alternatively have set 'male' to be the reference level, in which case males would be the default, and the female coefficient would have been around -3.23 (meaning that female blood pressure is 3.23 units lower than the male blood pressure at a fixed age).

When using a categorical variable as a predictor in a regression model, it is recoded into "dummy variables" (also known as "indicator variables"). A dummy variable for a single level, say `a`, of a variable `x`, is a variable that is equal to `1` when `x=a` and is equal to `0` when `x` is not equal to `a`. These dummy variables are included in the regression model, to represent the variable that they are derived from.

Statsmodels, like most software, will automatically recode a categorical variable into dummy variables, and will select a reference level (it is possible to override this choice, but we do not cover that here). When interpreting the regression output, the level that is omitted should be seen as having a coefficient of 0, with a standard error of 0. It is important to note that the selection of a reference level is arbitrary and does not imply a constraint on the model, or an assumption about the population that it is intended to capture.

5.5 A model with three variables

Next we add a third variable, body mass index (BMI), to the model. BMI is a measure that is used to assess if a person has healthy weight given their height. BMXBMI is the NHANES variable containing the BMI value for each subject.

[13]:
```
model = sm.OLS.from_formula("BPXSY1 ~ RIDAGEYR + BMXBMI + RIAGENDRx", data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.228
Model:                            OLS   Adj. R-squared:                  0.228
Method:                 Least Squares   F-statistic:                     502.0
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          8.54e-286
Time:                        15:01:15   Log-Likelihood:                -21461.
No. Observations:                5102   AIC:                         4.293e+04
Df Residuals:                    5098   BIC:                         4.296e+04
Df Model:                           3
Covariance Type:            nonrobust
=================================================================================
=====
                        coef    std err          t      P>|t|      [0.025
0.975]
--------------------------------------------------------------------------------
-----
Intercept            91.5840      1.198     76.456      0.000      89.236
93.932
RIAGENDRx[T.Male]     3.5783      0.457      7.833      0.000       2.683
4.474
RIDAGEYR              0.4709      0.013     36.582      0.000       0.446
0.496
BMXBMI                0.3060      0.033      9.351      0.000       0.242
0.370
==============================================================================
Omnibus:                      752.325   Durbin-Watson:                   2.040
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1776.087
Skew:                           0.847   Prob(JB):                         0.00
Kurtosis:                       5.343   Cond. No.                         316.
==============================================================================

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

Not surprisingly, BMI is positively associated with SBP. Given two subjects with the same gender and age, and whose BMI differs by 1 unit, the person with greater BMI will have, on average, 0.31 units greater systolic blood pressure (SBP). Also note that after adding BMI to the model, the coefficient for gender became somewhat greater. This is due to the fact that the three covariates in the model, age, gender, and BMI, are mutually correlated, as shown next:

[14]:

```
da[["RIDAGEYR", "RIAGENDR", "BMXBMI"]].corr()
```

[14]:

```
          RIDAGEYR  RIAGENDR    BMXBMI
RIDAGEYR  1.000000 -0.021398  0.023089
RIAGENDR -0.021398  1.000000  0.080463
BMXBMI    0.023089  0.080463  1.000000
```

Although the correlations among these three variables are not strong, they are sufficient to induce fairly substantial differences in the regression coefficients (e.g. the gender coefficient changes from 3.23 to 3.58). In this example, the gender effect becomes larger after we control for BMI - we can take this to mean that BMI was masking part of the association between gender and blood pressure. In other settings, including additional covariates can reduce the association between a covariate and an outcome.

6 Visualization of the fitted models

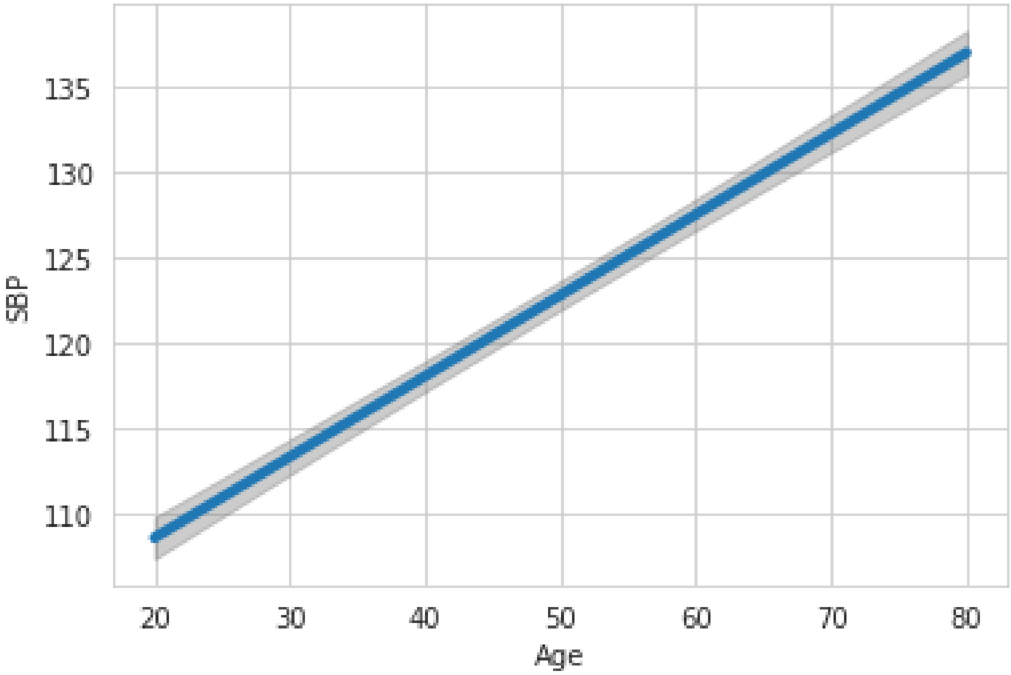
In this section we demonstrate some graphing techniques that can be used to gain a better understanding of a regression model that has been fit to data.

We start with plots that allow us to visualize the fitted regression function, that is, the mean systolic blood pressure expressed as a function of the covariates. These plots help to show the estimated role of one variable when the other variables are held fixed. We will also plot 95%

simultaneous confidence bands around these fitted lines. The estimated mean curve is never exactly correct, but we can be 95% confident that the true mean curve falls somewhere within the shaded regions of the plots below.

This type of plot requires us to fix the values of all variables other than the independent variable (SBP here), and one independent variable that we call the *focus variable* (which is age here). Below we fix the gender as "female" and the BMI as 25. Thus, the graphs below show the relationship between expected SBP and age for women with BMI equal to 25.

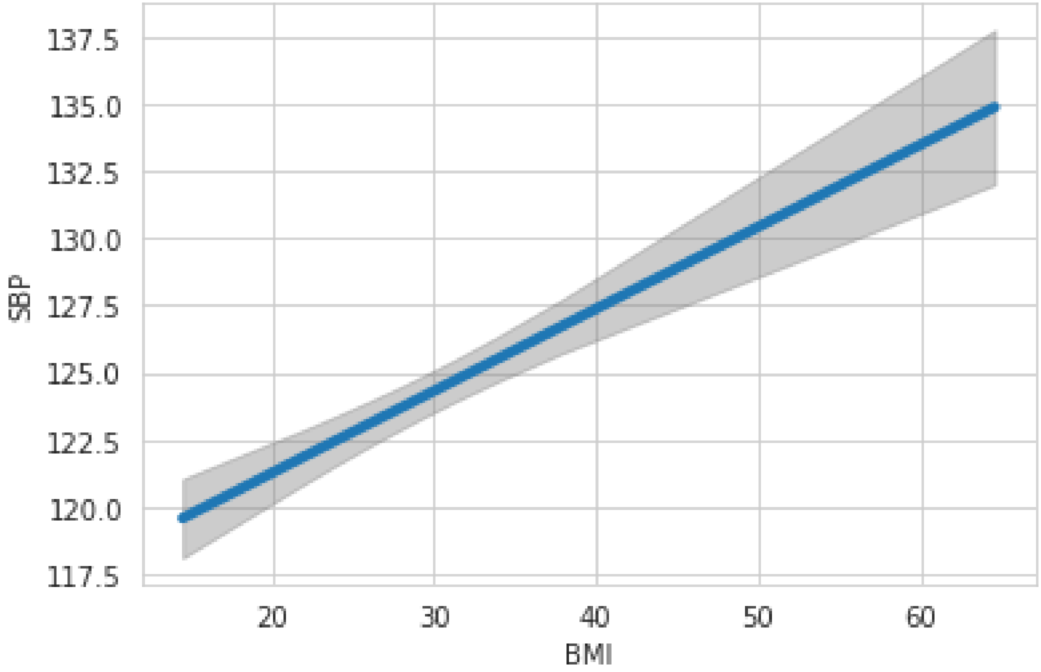
[15]:
```python
from statsmodels.sandbox.predict_functional import predict_functional

# Fix certain variables at reference values.  Not all of these
# variables are used here, but we provide them with a value anyway
# to prevent a warning message from appearing.
values = {"RIAGENDRx": "Female", "RIAGENDR": 2, "BMXBMI": 25,
          "DMDEDUC2": 1, "RIDRETH1": 1, "SMQ020": 1}

pr, cb, fv = predict_functional(result, "RIDAGEYR",
                values=values, ci_method="simultaneous")

sns.set_style("whitegrid")

ax = sns.lineplot(fv, pr, lw=4)
ax.fill_between(fv, cb[:, 0], cb[:, 1], color='grey', alpha=0.4)
ax.set_xlabel("Age")
_ = ax.set_ylabel("SBP")
```



The analogous plot for BMI is shown next. Here we fix the gender as “female” and the age at 50, so we are looking at the relationship between expected SBP and age for women of age 50.

[16]:

```
del values["BMXBMI"]
values["RIDAGEYR"] = 50
pr, cb, fv = predict_functional(result, "BMXBMI",
                values=values, ci_method="simultaneous")

sns.set_style("whitegrid")

ax = sns.lineplot(fv, pr, lw=4)
ax.fill_between(fv, cb[:, 0], cb[:, 1], color='grey', alpha=0.4)
ax.set_xlabel("BMI")
_ = ax.set_ylabel("SBP")
```



The error band for BMI is notably wider than the error band for age, indicating that there is less certainty about the relationsuip between BMI and SBP compared to the relationship between age and SBP. This is partly because the BMI values are less uniformly distributed. Very few subjects have BMI greater than 50, so we have less information from the data about the population mean, e.g. $E[y|a = 50, g]$ in this area. Since there is less information, the uncertainty is greater, hence the error bands are wider.

6.1 Visualizing variance structure

The discussion so far has primarily focused on the mean structure of the population, that is, the model for the average SBP of a person with a given age, gender, and BMI. A regression model can also be used to assess the *variance structure* of the population – that is, how much and in what manner the observations deviate from their mean. We will focus on informal, graphical methods for assessing this.

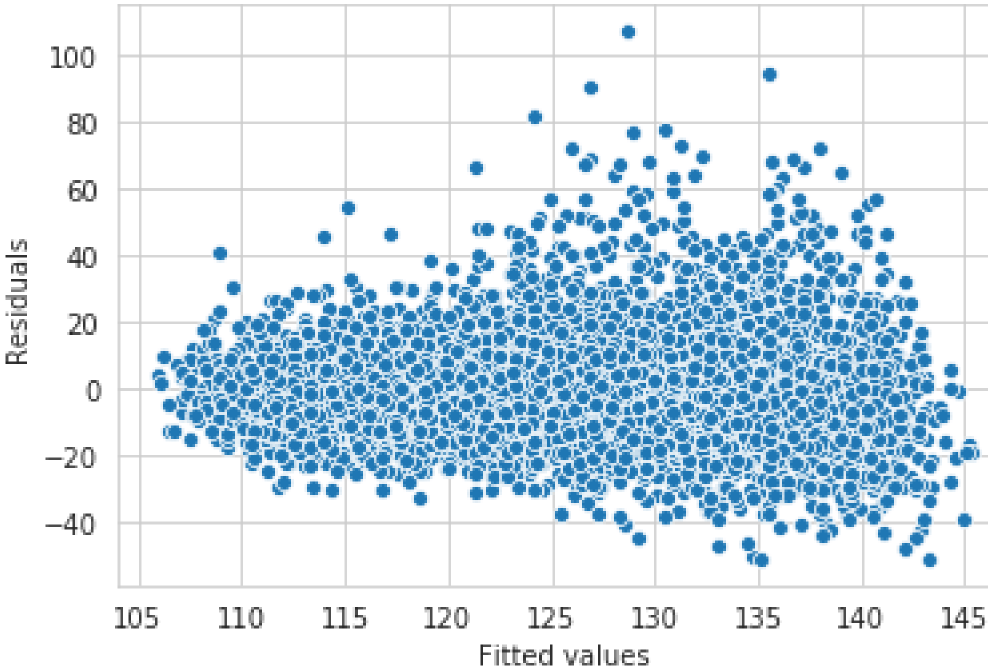
To begin with, we plot the residuals against the fitted values. Recall that the fitted values are the estimated means for each observation, and the residuals are the difference between an observation and its fitted mean. For example, the model may estimate that a 50 year old female will have on average an SBP of 125. But a specific 50 year old female may have a blood pressure of 110 or 150, for example. The fitted values for both of these women are 125, and their residuals are -15, and 25, respectively.

The simplest variance pattern that we can see in a linear regression occurs when the points are scattered around the mean, with the same degree of scatter throughout the range of the covariates. This is called *homoescedasticity*, or *constant variance*. When there are multiple covariates, it is hard to assess whether the variance is constant in this sense, but we can easily check for a "mean/variance relationship". This means that there is a systematic relationship between the variance and the mean, i.e. the variance either increases or decreases systematically with the mean. The plot of residuals on fitted values is used to assess whether such a mean/variance relationship is present.

Below we show the plot of residuals on fitted values for the NHANES data. It appears that we have a modestly increasing mean/variance relationship. That is, the scatter around the mean blood pressure is greater when the mean blood pressure itself is greater.

[17]:

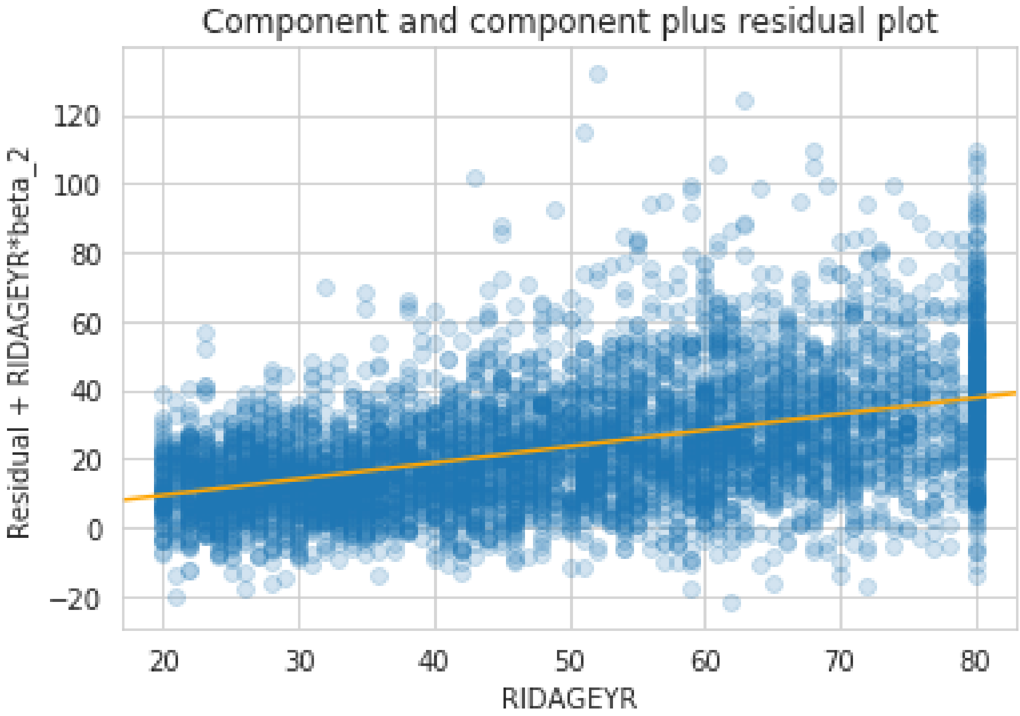
```
pp = sns.scatterplot(result.fittedvalues, result.resid)
pp.set_xlabel("Fitted values")
_ = pp.set_ylabel("Residuals")
```



A "component plus residual plot" or "partial residual plot" is intended to show how the data would look if all but one covariate could be fixed at reference values. By controlling the values of these covariates, all remaining variation is due either to the “focus variable” (the one variable that is left unfixed, and is plotted on the horizontal axis), or to sources of variation that are unexplained by any of our covariates.

For example, the partial residual plot below shows how age (horizontal axis) and SBP (vertical axis) would be related if gender and BMI were fixed. Note that the origin of the vertical axis in these plots is not meaningful (we are not implying that anyone’s blood pressure would be negative), but the differences along the vertical axis are meaningful. This plot implies that when BMI and gender are held fixed, the average blood pressures of an 80 and 18 year old differ by around 30 mm/Hg. This plot also shows, as discussed above, that the deviations from the mean are somewhat smaller at the low end of the range compared to the high end of the range. We also see that at the high end of the range, the deviations from the mean are somewhat right-skewed, with exceptionally high SBP values being more common than exceptionally low SBP values.

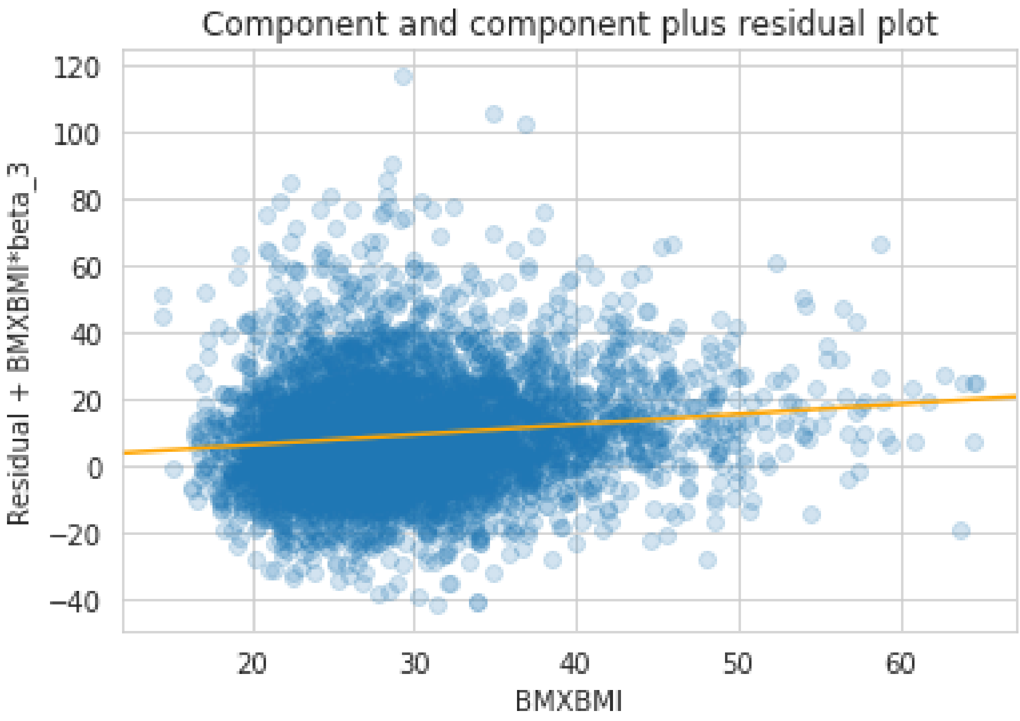
[18]:
```python
from statsmodels.graphics.regressionplots import plot_ccpr

plt.clf()
ax = plt.axes()
plot_ccpr(result, "RIDAGEYR", ax)
ax.lines[0].set_alpha(0.2) # Reduce overplotting with transparency
_ = ax.lines[1].set_color('orange')
```



Next we have a partial residual plot that shows how BMI (horizontal axis) and SBP (vertical axis) would be related if gender and age were fixed. Compared to the plot above, we see here that age is more uniformly distributed than BMI. Also, it appears that there is more scatter in the partial residuals for BMI compared to what we saw above for age. Thus there seems to be less information about SBP in BMI, although a trend certainly exists.

[19]:

```
ax = plt.axes()
plot_ccpr(result, "BMXBMI", ax)
ax.lines[0].set_alpha(0.2)
_ = ax.lines[1].set_color('orange')
```

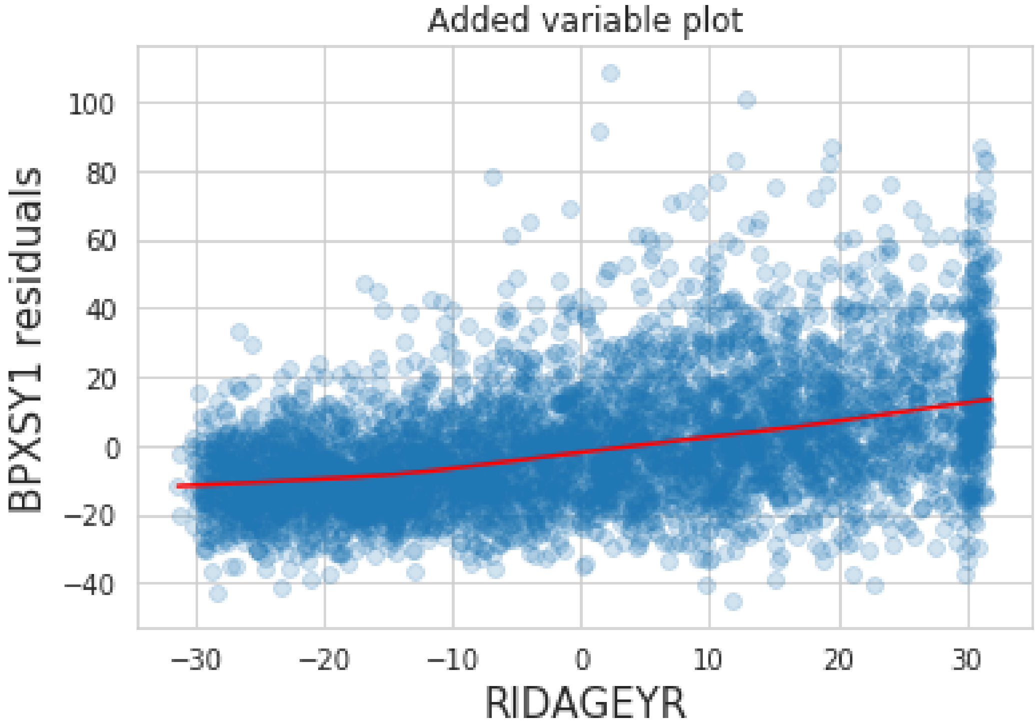


7 Assessing curvature

As noted above, a linear model is "linear" in an important technical sense, but this does not mean that linear regression can only be used to model linear phenomena. The models that we fit above are all linear in terms of the specified mean structure relationship between the covariates (age, etc.) and the response (blood pressure). To assess whether the data support this linear relationship, we can use an *added variable plot*. This is a diagnostic plot that aims to show how the response is related to one of the predictors, independently of how this relationship is specified in the model. Thus, although we have modeled the mean structure relationship between age (for example) and blood pressure as linear, the added variable plot will allow us to see if the actual relationship deviates from this form.

The cell below shows the added variable plot for age in a model including main effects for age, BMI, and gender. Note that we are using the GLM function here to fit the model. GLM is a more general class of regression procedures that includes linear regression (OLS) as a special case. OLS is the default for GLM, so the code below fits the identical model as fit above with the OLS function. Currently, it is necessary to use GLM when fitting linear models if we want to produce added variable plots.

[20]:
```
from statsmodels.graphics.regressionplots import add_lowess

model = sm.GLM.from_formula("BPXSY1 ~ RIDAGEYR + BMXBMI + RIAGENDRx", data=da)
result = model.fit()

fig = result.plot_added_variable("RIDAGEYR")
fig.axes[0].lines[0].set_alpha(0.2)
_ = add_lowess(fig.axes[0], frac=0.5)
```



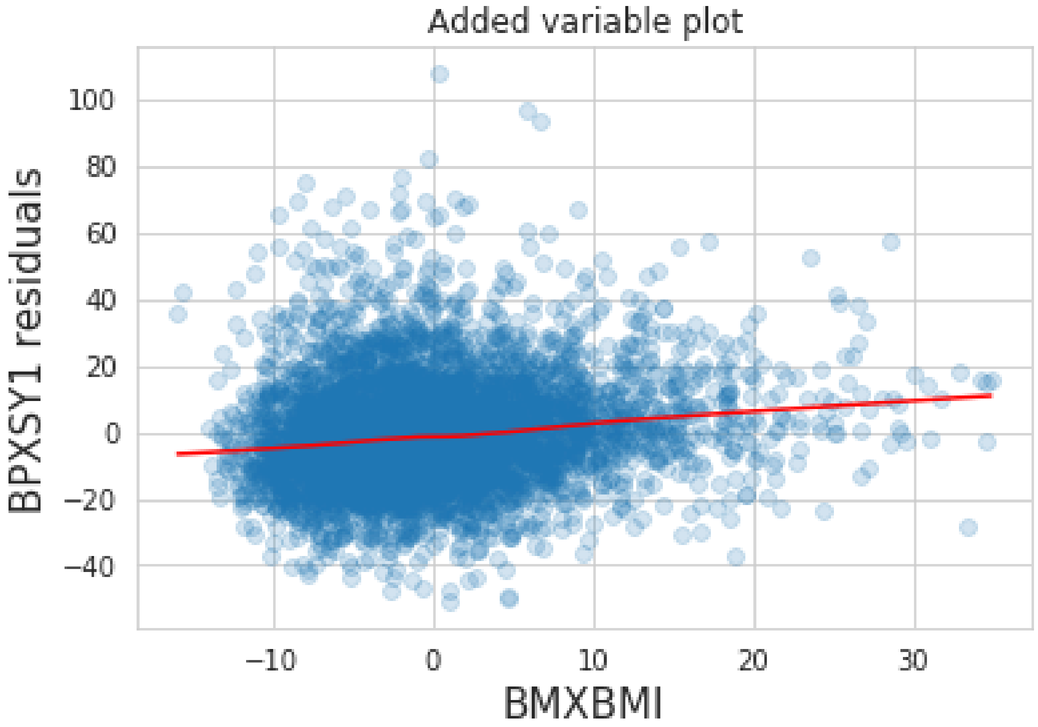
The plot above suggests that the increasing trend identified by the linear model is approximately correct, but that the true relationship may be slightly nonlinear, with positive curvature. This means that the annual mean increment in blood pressure may get larger as people age.

We won't get into the mathematical details of how added variable plots are constructed, but we note that the construction involves residualization. Therefore, the "focus variable" (age above) is centered relative to its mean in the plot.

As another example, below is the added variable plot for BMI:

[21]:
```
from statsmodels.graphics.regressionplots import add_lowess

model = sm.GLM.from_formula("BPXSY1 ~ RIDAGEYR + BMXBMI + RIAGENDRx", data=da)
result = model.fit()
```

```
fig = result.plot_added_variable("BMXBMI")
fig.axes[0].lines[0].set_alpha(0.2)
_ = add_lowess(fig.axes[0], frac=0.5)
```



8 Basis functions and splines

If we have identified possible nonlinear relationships that we would like to include in a model, one way to accomplish this while remaining within the framework of linear regression is to use basis functions. A collection of basis functions is any collection of functions that we can evaluate using one or more of the covariates in a model. For example, we may consider the polynomial basis functions $x, x^2, \ldots$. We can evaluate these polynomials using age, yielding $\text{age}, \text{age}^2, \ldots$. These variables can then be included in the mean structure of the regression model:

$$E[\text{SBP} \mid \text{age}, \text{BMI}] = b_0 + b_1 \cdot \text{age} + b_2 \cdot \text{age}^2 + b_3 \cdot \text{BMI}.$$

Note that this is still a linear model, since we can treat age^2 as simply being another covariate (like BMI) that we have added to the model. Thus, all of the techniques used for working with linear models remain applicable here, although we are now able to capture nonlinear relationships in the mean structure. Also note that above we included a polynomial (quadratic) term for age, but it would be possible to simultaneously add polynomial terms for several terms in the model (e.g. for both age and BMI).

[22]:

```python
da["RIDAGEYR_z"] = (da.RIDAGEYR - da.RIDAGEYR.mean()) / da.RIDAGEYR.std()
fml = "BPXSY1 ~ RIDAGEYR_z + I(RIDAGEYR_z**2) + RIAGENDRx"
model = sm.OLS.from_formula(fml, data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.215
Model:                            OLS   Adj. R-squared:                  0.214
Method:                 Least Squares   F-statistic:                     465.1
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          4.21e-267
Time:                        15:01:25   Log-Likelihood:                -21505.
No. Observations:                5102   AIC:                         4.302e+04
Df Residuals:                    5098   BIC:                         4.304e+04
Df Model:                           3
Covariance Type:            nonrobust
================================================================================
======
                         coef    std err          t      P>|t|      [0.025
0.975]
--------------------------------------------------------------------------------
------
Intercept            123.8813      0.404    306.776      0.000     123.090
124.673
RIAGENDRx[T.Male]      3.2319      0.459      7.039      0.000       2.332
4.132
RIDAGEYR_z             8.3594      0.231     36.185      0.000       7.907
8.812
I(RIDAGEYR_z ** 2)     0.1859      0.248      0.750      0.453      -0.300
0.672
==============================================================================
Omnibus:                      708.996   Durbin-Watson:                   2.036
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1594.809
Skew:                           0.819   Prob(JB):                         0.00
Kurtosis:                       5.196   Cond. No.                         3.93
==============================================================================

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

As seen above, the coefficient for age^2 is not significantly different from zero. This is not the only arbiter of whether there is curvature in the mean relationship between blood pressure and age, but it does indicate that we are unable to estimate any curvature in these data.

Polynomial basis function are easy to explain, but have been criticized for being too “global” and for inducing collinearity. The term “global” in this context means that the fitted value at one point x in the covariate space may depend in unexpected ways on observations (y', x') for points

x' that are far from x. A very popular family of basis functions that avoid this issue are the various *spline* families, which are local polynomials.

[23]:

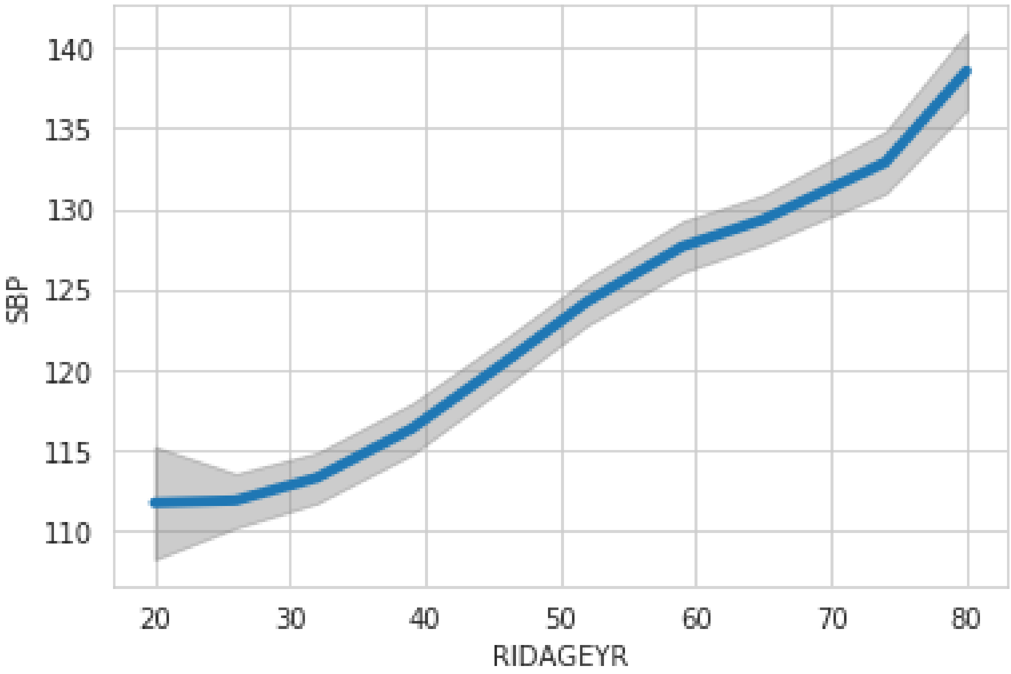
```
model = sm.OLS.from_formula("BPXSY1 ~ bs(RIDAGEYR, 5) + BMXBMI + RIAGENDRx",␣
  ↪data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.231
Model:                            OLS   Adj. R-squared:                  0.230
Method:                 Least Squares   F-statistic:                     219.0
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          2.76e-285
Time:                        15:01:25   Log-Likelihood:                -21451.
No. Observations:                5102   AIC:                         4.292e+04
Df Residuals:                    5094   BIC:                         4.297e+04
Df Model:                           7
Covariance Type:            nonrobust
================================================================================
======
                         coef    std err          t      P>|t|      [0.025
0.975]
--------------------------------------------------------------------------------
------
Intercept            103.6601      1.536     67.468      0.000     100.648
106.672
RIAGENDRx[T.Male]      3.6039      0.456      7.900      0.000       2.710
4.498
bs(RIDAGEYR, 5)[0]    -0.5552      2.268     -0.245      0.807      -5.002
3.891
bs(RIDAGEYR, 5)[1]     3.0907      1.575      1.962      0.050       0.002
6.179
bs(RIDAGEYR, 5)[2]    19.1714      2.124      9.024      0.000      15.007
23.336
bs(RIDAGEYR, 5)[3]    17.7960      1.762     10.099      0.000      14.341
21.251
bs(RIDAGEYR, 5)[4]    26.8944      1.498     17.955      0.000      23.958
29.831
BMXBMI                 0.3210      0.033      9.729      0.000       0.256
0.386
==============================================================================
Omnibus:                      745.462   Durbin-Watson:                   2.037
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1773.011
Skew:                           0.837   Prob(JB):                         0.00
Kurtosis:                       5.353   Cond. No.                         459.
==============================================================================
Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
```

Below we plot the fitted mean curve, which is an estimate of $E[\text{SBP}|\text{age}, \text{gender} = F, \text{BMI} = 25]$, along with a 95% simultaneous confidence band to assess the uncertainty.

[24]:

```
del da["RIDAGEYR_z"]
values = {"RIAGENDRx": "Female", "RIAGENDR": 2, "BMXBMI": 25,
          "DMDEDUC2": 1, "RIDRETH1": 1, "SMQ020": 1}

pr, cb, fv = predict_functional(result, "RIDAGEYR",
                values=values, ci_method="simultaneous")

sns.set_style("whitegrid")
ax = sns.lineplot(fv, pr, lw=4)
ax.fill_between(fv, cb[:, 0], cb[:, 1], color='grey', alpha=0.4)
ax.set_xlabel("RIDAGEYR")
_ = ax.set_ylabel("SBP")
```



9 Interactions

The basic linear models we fit above are *additive*, meaning that the change in the expected response associated with a change in one covariate is not dependent on the values of the other covariates. In the setting of a regression model with two covariates, additivity implies that the value of

$$E[y|x_1 = a + 1, x_2 = x] - E[y|x_1 = a, x_2 = x]$$

does not depend on x. In the blood pressure example, additivity would imply that the difference in mean blood pressure between a 50 year-old woman and a 40 year-old woman is the same as the difference in mean blood pressure between a 50 year-old man and a 40 year-old man. In fact, this may not be the case.

We now return to modeling the SBP as predicted by age and BMI, including here an *interaction* between age and gender in the model. This interaction allows us to explore non-additivity between these variables. Note that while nonlinearities and interactions can be considered jointly, for simplicity we have removed the nonlinear part of the model (the basis splines) so we can focus only on the interaction.

Note that here we have centered the age variable. While not strictly required, there are several advantages to centering quantitative variables that are part of an interaction term in a regression model. One specific advantage is that the main effects for the variables in the interaction (here age and gender) are interpretable as the effects of one of these variable while holding the other variable fixed at its mean. For example, the main effect for gender in the model below is the difference in mean blood pressure between women and men who are at the mean age of the sample.

[25]:

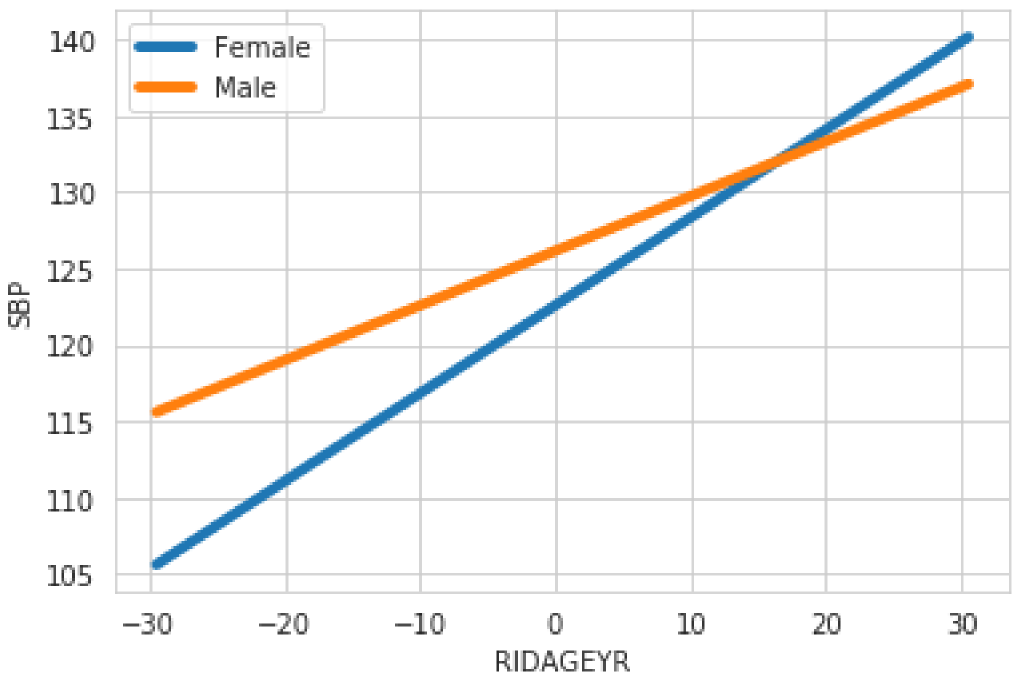
```
da["RIDAGEYR_cen"] = da.RIDAGEYR - da.RIDAGEYR.mean()
model = sm.OLS.from_formula("BPXSY1 ~ RIDAGEYR_cen*RIAGENDRx + BMXBMI", data=da)
result = model.fit()
print(result.summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                 BPXSY1   R-squared:                       0.239
Model:                            OLS   Adj. R-squared:                  0.238
Method:                 Least Squares   F-statistic:                     400.0
Date:                Mon, 27 Jan 2020   Prob (F-statistic):          4.37e-300
Time:                        15:01:26   Log-Likelihood:                -21425.
No. Observations:                5102   AIC:                         4.286e+04
Df Residuals:                    5097   BIC:                         4.289e+04
Df Model:                           4
Covariance Type:            nonrobust
================================================================================
==================
                                     coef    std err          t      P>|t|
[0.025      0.975]
--------------------------------------------------------------------------------
------------------
Intercept                        115.0502      1.026    112.149      0.000
113.039     117.061
RIAGENDRx[T.Male]                  3.5785      0.454      7.889      0.000
2.689       4.468
RIDAGEYR_cen                       0.5766      0.018     32.394      0.000
0.542       0.611
RIDAGEYR_cen:RIAGENDRx[T.Male]    -0.2182      0.026     -8.533      0.000
-0.268      -0.168
```

```
BMXBMI                             0.3013      0.032      9.273      0.000
0.238       0.365
==============================================================================
Omnibus:                      773.113   Durbin-Watson:                   2.040
Prob(Omnibus):                  0.000   Jarque-Bera (JB):             1861.274
Skew:                           0.861   Prob(JB):                         0.00
Kurtosis:                       5.406   Cond. No.                         139.
==============================================================================

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

The results shown above show that the main effects and interactions are all statistically significant, which suggests that the roles of age and gender with respect to blood pressure may not be additive. Men have a higher intercept but lower slope than women. The easiest way to see what this tells us is through a graph:

[26]:
```
values["RIAGENDRx"] = "Female"
values["RIDAGEYR"] = np.nan
pr1, cb1, fv1 = predict_functional(result, "RIDAGEYR_cen",
                values=values, ci_method="simultaneous")

sns.set_style("whitegrid")
ax = sns.lineplot(fv1, pr1, lw=4, label="Female")

values["RIAGENDRx"] = "Male"
pr2, cb2, fv2 = predict_functional(result, "RIDAGEYR_cen",
                values=values, ci_method="simultaneous")
ax = sns.lineplot(fv2, pr2, lw=4, label="Male")

ax.set_xlabel("RIDAGEYR")
_ = ax.set_ylabel("SBP")
```


Female
Male
140
135
130
125
120
115
110
105
SBP
−30
−20
−10
0
10
20
30
RIDAGEYR