Chapter_7_Non_Linear_Modeling

April 2, 2024

In this lab, we demonstrate some of the nonlinear models discussed in this chapter. We use the Wage data as a running example, and show that many of the complex non-linear ftting procedures discussed can easily be implemented in Python.

[1]:
```
import numpy as np, pandas as pd
from matplotlib.pyplot import subplots
import statsmodels.api as sm
from ISLP import load_data
from ISLP.models import (summarize,poly,ModelSpec as MS)
from statsmodels.stats.anova import anova_lm
```

We again collect the new imports needed for this lab. Many of these are developed specifcally for the ISLP package.

[2]:
```
from pygam import (s as s_gam,l as l_gam,f as f_gam,LinearGAM,LogisticGAM)
from ISLP.transforms import (BSpline,NaturalSpline)
from ISLP.models import bs, ns
from ISLP.pygam import (approx_lam,degrees_of_freedom,plot as plot_gam,anova as␣
↪anova_gam)
```

0.1 7.8.1 Polynomial Regression and Step Functions

We start by demonstrating how Figure 7.1 can be reproduced. Let's begin by loading the data.

[3]:
```
Wage = load_data('Wage')
y = Wage['wage']
age = Wage['age']
```

Throughout most of this lab, our response is Wage['wage'], which we have stored as y above. As in Section 3.6.6, we will use the poly() function to create a model matrix that will ft a 4th degree polynomial in age.

[4]:
```
poly_age = MS([poly('age', degree=4)]).fit(Wage)
M = sm.OLS(y, poly_age.transform(Wage)).fit()
summarize(M)
```

[4]:

	coef	std err	t	P>|t|
intercept	111.7036	0.729	153.283	0.000
poly(age, degree=4)[0]	447.0679	39.915	11.201	0.000
poly(age, degree=4)[1]	-478.3158	39.915	-11.983	0.000

```
poly(age, degree=4)[2]  125.5217   39.915    3.145  0.002
poly(age, degree=4)[3]  -77.9112   39.915   -1.952  0.051
```

This polynomial is constructed using the function poly(), which creates a special transformer Poly() (using sklearn terminology for feature transformations such as PCA() seen in Section 6.5.3) which allows for easy evaluation of the polynomial at new data points. Here poly() is referred to as a helper function, and sets up the transformation; Poly() is the actual workhorse that computes the transformation. See also the discussion of transformations on page 118

In the code above, the frst line executes the fit() method using the dataframe Wage. This recomputes and stores as attributes any parameters needed by Poly() on the training data, and these will be used on all subsequent evaluations of the transform() method. For example, it is used on the second line, as well as in the plotting function developed below.

We now create a grid of values for age at which we want predictions.

[5]:
```
age_grid = np.linspace(age.min(),age.max(),100)
age_df = pd.DataFrame({'age': age_grid})
```

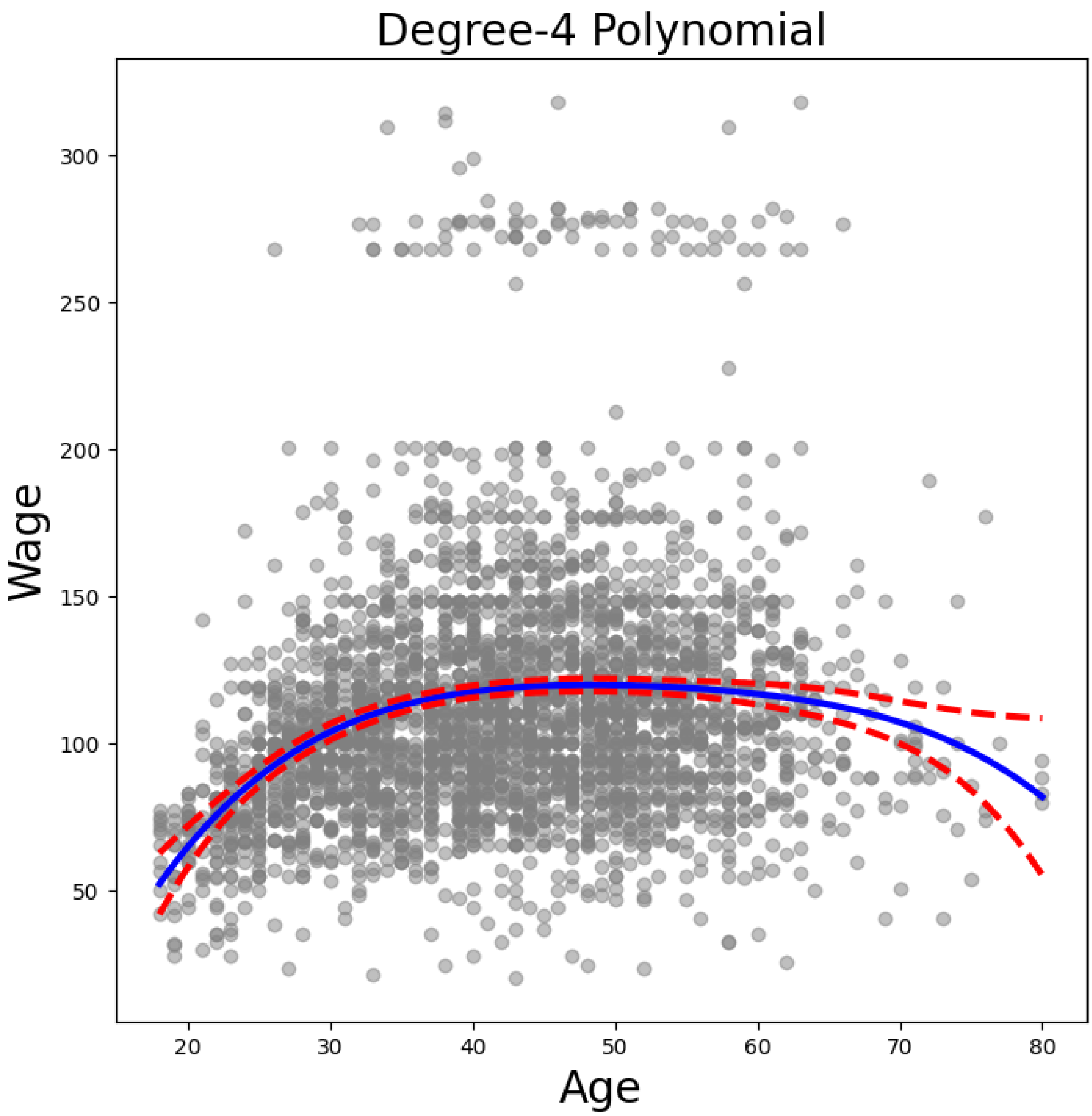
Finally, we wish to plot the data and add the ft from the fourth-degree polynomial. As we will make several similar plots below, we frst write a function to create all the ingredients and produce the plot. Our function takes in a model specifcation (here a basis specifed by a transform), as well as a grid of age values. The function produces a ftted curve as well as 95% confdence bands. By using an argument for basis we can produce and plot the results with several diferent transforms, such as the splines we will see shortly.

[6]:
```
def plot_wage_fit(age_df,basis,title):
    X = basis.transform(Wage)
    Xnew = basis.transform(age_df)
    M = sm.OLS(y, X).fit()
    preds = M.get_prediction(Xnew)
    bands = preds.conf_int(alpha=0.05)
    fig, ax = subplots(figsize=(8,8))
    ax.scatter(age,y,facecolor='gray',alpha=0.5)
    for val, ls in zip([preds.predicted_mean ,bands[:,0],bands[:
 ↪,1]],['b','r--','r--']):
        ax.plot(age_df.values, val, ls, linewidth=3)
    ax.set_title(title, fontsize=20)
    ax.set_xlabel('Age', fontsize=20)
    ax.set_ylabel('Wage', fontsize=20);
    return ax
```

We include an argument alpha to ax.scatter() to add some transparency to the points. This provides a visual indication of density. Notice the use of the zip() function in the for loop above (see Section 2.3.8). We have three lines to plot, each with diferent colors and line types. Here zip() conveniently bundles these together as iterators in the loop.

We now plot the ft of the fourth-degree polynomial using this function.

[7]:
```
plot_wage_fit(age_df,poly_age,'Degree-4 Polynomial');
```



With polynomial regression we must decide on the degree of the polynomial to use. Sometimes we just wing it, and decide to use second or third degree polynomials, simply to obtain a nonlinear ft. But we can make such a decision in a more systematic way. One way to do this is through hypothesis tests, which we demonstrate here. We now ft a series of models ranging from linear (degree-one) to degree-fve polynomials, and look to determine the simplest model that is sufcient to explain the relationship between wage and age. We use the anova_lm() function, which performs a series of ANOVA tests. An analysis of variance or ANOVA tests the null hypothesis analysis of variance that a model M1 is sufcient to explain the data against the alternative hypothesis that a more complex model M2 is required. The determination is based on an F-test. To perform the test, the models M1 and M2 must be nested: the space spanned by the predictors in M1 must be a subspace of the space spanned by the predictors in M2. In this case, we ft fve different polynomial models and sequentially compare the simpler model to the more complex model.

[8]:
```python
models = [MS([poly('age', degree=d)]) for d in range(1, 6)]
Xs = [model.fit_transform(Wage) for model in models]
anova_lm(*[sm.OLS(y, X_).fit() for X_ in Xs])
```

[8]:

	df_resid	ssr	df_diff	ss_diff	F	Pr(>F)
0	2998.0	5.022216e+06	0.0	NaN	NaN	NaN
1	2997.0	4.793430e+06	1.0	228786.010128	143.593107	2.363850e-32
2	2996.0	4.777674e+06	1.0	15755.693664	9.888756	1.679202e-03
3	2995.0	4.771604e+06	1.0	6070.152124	3.809813	5.104620e-02
4	2994.0	4.770322e+06	1.0	1282.563017	0.804976	3.696820e-01

Notice the * in the anova_lm() line above. This function takes a variable number of non-keyword arguments, in this case ftted models. When these models are provided as a list (as is done here), it must be prefxed by *.

The p-value comparing the linear models[0] to the quadratic models[1] is essentially zero, indicating that a linear ft is not sufcient.8 Similarly the p-value comparing the quadratic models[1] to the cubic models[2] is very low (0.0017), so the quadratic ft is also insufcient. The p-value comparing the cubic and degree-four polynomials, models[2] and models[3], is approximately 5%, while the degree-fve polynomial models[4] seems unnecessary because its p-value is 0.37. Hence, either a cubic or a quartic polynomial appear to provide a reasonable ft to the data, but lower- or higher-order models are not justifed.

In this case, instead of using the anova() function, we could have obtained these p-values more succinctly by exploiting the fact that poly() creates orthogonal polynomials.

[9]:
```python
summarize(M)
```

[9]:

	coef	std err	t	P>|t|
intercept	111.7036	0.729	153.283	0.000
poly(age, degree=4)[0]	447.0679	39.915	11.201	0.000
poly(age, degree=4)[1]	-478.3158	39.915	-11.983	0.000
poly(age, degree=4)[2]	125.5217	39.915	3.145	0.002
poly(age, degree=4)[3]	-77.9112	39.915	-1.952	0.051

Notice that the p-values are the same, and in fact the square of the t-statistics are equal to the F-statistics from the anova_lm() function; for example:

[10]:
```python
(-11.983)**2
```

[10]: 143.59228900000002

However, the ANOVA method works whether or not we used orthogonal polynomials, provided the models are nested. For example, we can use anova_lm() to compare the following three models, which all have a linear term in education and a polynomial in age of diferent degrees:

[11]:
```python
models = [MS(['education', poly('age', degree=d)]) for d in range(1, 4)]
XEs = [model.fit_transform(Wage) for model in models]
anova_lm(*[sm.OLS(y, X_).fit() for X_ in XEs])
```

[11]:

	df_resid	ssr	df_diff	ss_diff	F	Pr(>F)
0	2997.0	3.902335e+06	0.0	NaN	NaN	NaN
1	2996.0	3.759472e+06	1.0	142862.701185	113.991883	3.838075e-26
2	2995.0	3.753546e+06	1.0	5926.207070	4.728593	2.974318e-02

As an alternative to using hypothesis tests and ANOVA, we could choose the polynomial degree using cross-validation, as discussed in Chapter 5.

Next we consider the task of predicting whether an individual earns more than $250,000 per year. We proceed much as before, except that frst we create the appropriate response vector, and then apply the glm() function using the binomial family in order to ft a polynomial logistic regression model

[12]:
```
X = poly_age.transform(Wage)
high_earn = Wage['high_earn'] = y > 250 # shorthand
glm = sm.GLM(y > 250,X,family=sm.families.Binomial())
B = glm.fit()
summarize(B)
```

[12]:

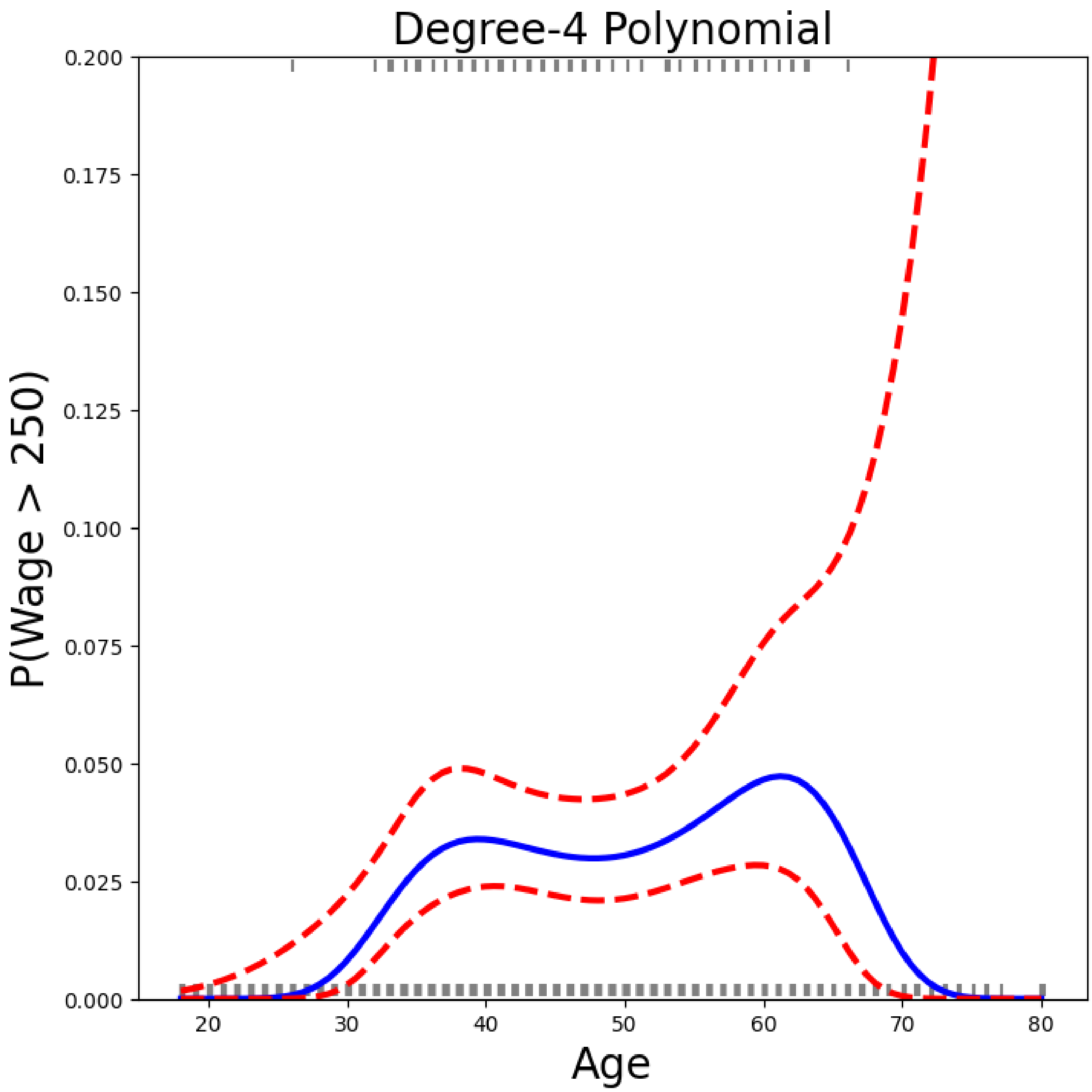
	coef	std err	z	P>|z|
intercept	-4.3012	0.345	-12.457	0.000
poly(age, degree=4)[0]	71.9642	26.133	2.754	0.006
poly(age, degree=4)[1]	-85.7729	35.929	-2.387	0.017
poly(age, degree=4)[2]	34.1626	19.697	1.734	0.083
poly(age, degree=4)[3]	-47.4008	24.105	-1.966	0.049

Once again, we make predictions using the get_prediction() method.

[13]:
```
newX = poly_age.transform(age_df)
preds = B.get_prediction(newX)
bands = preds.conf_int(alpha=0.05)
```

We now plot the estimated relationship.

[14]:
```
fig, ax = subplots(figsize=(8,8))
rng = np.random.default_rng(0)
ax.scatter(age +0.2 * rng.uniform(size=y.shape[0]),np.where(high_earn, 0.198, 0.
 ↪002),fc='gray',marker='|')
for val, ls in zip([preds.predicted_mean ,bands[:,0],bands[:
 ↪,1]],['b','r--','r--']):
    ax.plot(age_df.values, val, ls, linewidth=3)
ax.set_title('Degree-4 Polynomial', fontsize=20)
ax.set_xlabel('Age', fontsize=20)
ax.set_ylim([0,0.2])
ax.set_ylabel('P(Wage > 250)', fontsize=20);
```



We have drawn the age values corresponding to the observations with wage values above 250 as gray marks on the top of the plot, and those with wage values below 250 are shown as gray marks on the bottom of the plot. We added a small amount of noise to jitter the age values a bit so that observations with the same age value do not cover each other up. This type of plot is often called a rug plot.

In order to ft a step function, as discussed in Section 7.2, we frst use the pd.qcut() function to discretize age based on quantiles. Then we use pd.get_dummies() to create the columns of the model matrix for this categorical variable. Note that this function will include all columns for a given categorical, rather than the usual approach which drops one of the levels.

[15]:
```
cut_age = pd.qcut(age, 4)
summarize(sm.OLS(y, pd.get_dummies(cut_age)).fit())
```

[15]:

	coef	std err	t	P>|t|
(17.999, 33.75]	94.1584	1.478	63.692	0.0
(33.75, 42.0]	116.6608	1.470	79.385	0.0
(42.0, 51.0]	119.1887	1.416	84.147	0.0
(51.0, 80.0]	116.5717	1.559	74.751	0.0

Here pd.qcut() automatically picked the cutpoints based on the quantiles 25%, 50% and 75%, which results in four regions. We could also have specifed our own quantiles directly instead of the argument 4. For cuts not based on quantiles we would use the pd.cut() function. The function pd.qcut() (and pd.cut()) returns an ordered categorical variable. The regression model then creates a set of dummy variables for use in the regression. Since age is the only variable in the model, the value $94,158.40 is the average salary for those under 33.75 years of age, and the other coefcients are the average salary for those in the other age groups. We can produce predictions and plots just as we did in the case of the polynomial ft.

0.2 7.8.2 Splines

In order to ft regression splines, we use transforms from the ISLP package. The actual spline evaluation functions are in the scipy.interpolate package; we have simply wrapped them as transforms similar to Poly() and PCA().

In Section 7.4, we saw that regression splines can be ft by constructing an appropriate matrix of basis functions. The BSpline() function generates the entire matrix of basis functions for splines with the specifed set of knots. By default, the B-splines produced are cubic. To change the degree, use the argument degree.

[16]:
```
bs_ = BSpline(internal_knots=[25,40,60], intercept=True).fit(age)
bs_age = bs_.transform(age)
bs_age.shape
```

[16]: (3000, 7)

This results in a seven-column matrix, which is what is expected for a cubicspline basis with 3 interior knots. We can form this same matrix using the bs() object, which facilitates adding this to a model-matrix builder (as in poly() versus its workhorse Poly()) described in Section 7.8.1.

We now ft a cubic spline model to the Wage data.

[17]:
```
bs_age = MS([bs('age', internal_knots=[25,40,60])])
Xbs = bs_age.fit_transform(Wage)
M = sm.OLS(y, Xbs).fit()
summarize(M)
```

[17]:

	coef	std err	t	P>|t|
intercept	60.4937	9.460	6.394	0.000
bs(age, internal_knots=[25, 40, 60])[0]	3.9805	12.538	0.317	0.751
bs(age, internal_knots=[25, 40, 60])[1]	44.6310	9.626	4.636	0.000
bs(age, internal_knots=[25, 40, 60])[2]	62.8388	10.755	5.843	0.000
bs(age, internal_knots=[25, 40, 60])[3]	55.9908	10.706	5.230	0.000
bs(age, internal_knots=[25, 40, 60])[4]	50.6881	14.402	3.520	0.000

```
bs(age, internal_knots=[25, 40, 60])[5]  16.6061   19.126  0.868  0.385
```

The column names are a little cumbersome, and have caused us to truncate the printed summary. They can be set on construction using the name argument as follows.

[18]:
```
bs_age = MS([bs('age',internal_knots=[25,40,60],name='bs(age)')])
Xbs = bs_age.fit_transform(Wage)
M = sm.OLS(y, Xbs).fit()
summarize(M)
```

[18]:
```
               coef  std err      t  P>|t|
intercept   60.4937    9.460  6.394  0.000
bs(age)[0]   3.9805   12.538  0.317  0.751
bs(age)[1]  44.6310    9.626  4.636  0.000
bs(age)[2]  62.8388   10.755  5.843  0.000
bs(age)[3]  55.9908   10.706  5.230  0.000
bs(age)[4]  50.6881   14.402  3.520  0.000
bs(age)[5]  16.6061   19.126  0.868  0.385
```

Notice that there are 6 spline coefcients rather than 7. This is because, by default, bs() assumes intercept=False, since we typically have an overall intercept in the model. So it generates the spline basis with the given knots, and then discards one of the basis functions to account for the intercept.

We could also use the df (degrees of freedom) option to specify the complexity of the spline. We see above that with 3 knots, the spline basis has 6 columns or degrees of freedom. When we specify df=6 rather than the actual knots, bs() will produce a spline with 3 knots chosen at uniform quantiles of the training data. We can see these chosen knots most easily using Bspline() directly:

[19]:
```
BSpline(df=6).fit(age).internal_knots_
```

[19]:
```
array([33.75, 42.  , 51.  ])
```

When asking for six degrees of freedom, the transform chooses knots at ages 33.75, 42.0, and 51.0, which correspond to the 25th, 50th, and 75th percentiles of age.

When using B-splines we need not limit ourselves to cubic polynomials (i.e. degree=3). For instance, using degree=0 results in piecewise constant functions, as in our example with pd.qcut() above.

[20]:
```
bs_age0 = MS([bs('age',df=3,degree=0)]).fit(Wage)
Xbs0 = bs_age0.transform(Wage)
summarize(sm.OLS(y, Xbs0).fit())
```

[20]:
```
                             coef  std err       t  P>|t|
intercept                 94.1584    1.478  63.687    0.0
bs(age, df=3, degree=0)[0]  22.3490    2.152  10.388    0.0
bs(age, df=3, degree=0)[1]  24.8076    2.044  12.137    0.0
bs(age, df=3, degree=0)[2]  22.7814    2.087  10.917    0.0
```

This ft should be compared with cell [15] where we use qcut() to create four bins by cutting at the 25%, 50% and 75% quantiles of age. Since we specifed df=3 for degree-zero splines here, there will also be knots at the same three quantiles. Although the coefcients appear diferent, we see that this is a result of the diferent coding. For example, the frst coefcient is identical in both cases, and is the mean response in the frst bin. For the second coefcient, we have $94.158 + 22.349 = 116.507$ 116.611, the latter being the mean in the second bin in cell [15]. Here the intercept is coded by a column of ones, so the second, third and fourth coefcients are increments for those bins. Why is the sum not exactly the same? It turns out that the qcut() uses , while bs() uses $<$ when deciding bin membership.

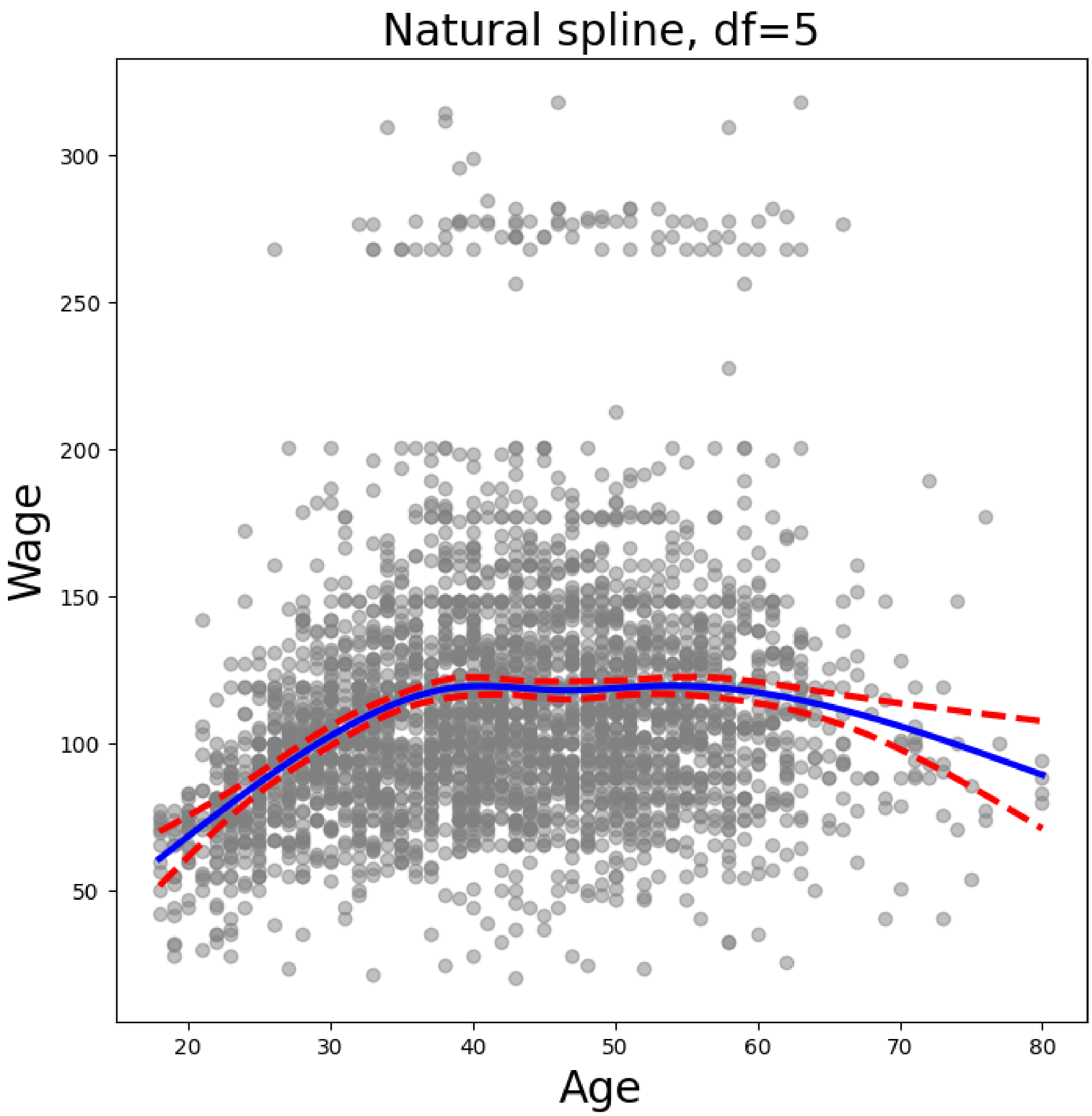
In order to ft a natural spline, we use the NaturalSpline() transform with the corresponding helper ns(). Here we ft a natural spline with fve degrees of freedom (excluding the intercept) and plot the results.

[21]:
```
ns_age = MS([ns('age', df=5)]).fit(Wage)
M_ns = sm.OLS(y, ns_age.transform(Wage)).fit()
summarize(M_ns)
```

[21]:

	coef	std err	t	P>|t|
intercept	60.4752	4.708	12.844	0.000
ns(age, df=5)[0]	61.5267	4.709	13.065	0.000
ns(age, df=5)[1]	55.6912	5.717	9.741	0.000
ns(age, df=5)[2]	46.8184	4.948	9.463	0.000
ns(age, df=5)[3]	83.2036	11.918	6.982	0.000
ns(age, df=5)[4]	6.8770	9.484	0.725	0.468

[22]:
```
plot_wage_fit(age_df,ns_age,'Natural spline, df=5');
```



0.3 7.8.3 Smoothing Splines and GAMs

A smoothing spline is a special case of a GAM with squared-error loss and a single feature. To ft GAMs in Python we will use the pygam package which can be installed via pip install pygam. The estimator LinearGAM() uses squared-error loss. The GAM is specifed by associating each column of a model matrix with a particular smoothing operation: s for smoothing spline; l for linear, and f for factor or categorical variables. The argument 0 passed to s below indicates that this smoother will apply to the frst column of a feature matrix. Below, we pass it a matrix with a single column: X_age. The argument lam is the penalty parameter   as discussed in Section 7.5.2.

[23]:
```
X_age = np.asarray(age).reshape((-1,1))
gam = LinearGAM(s_gam(0, lam=0.6))
```

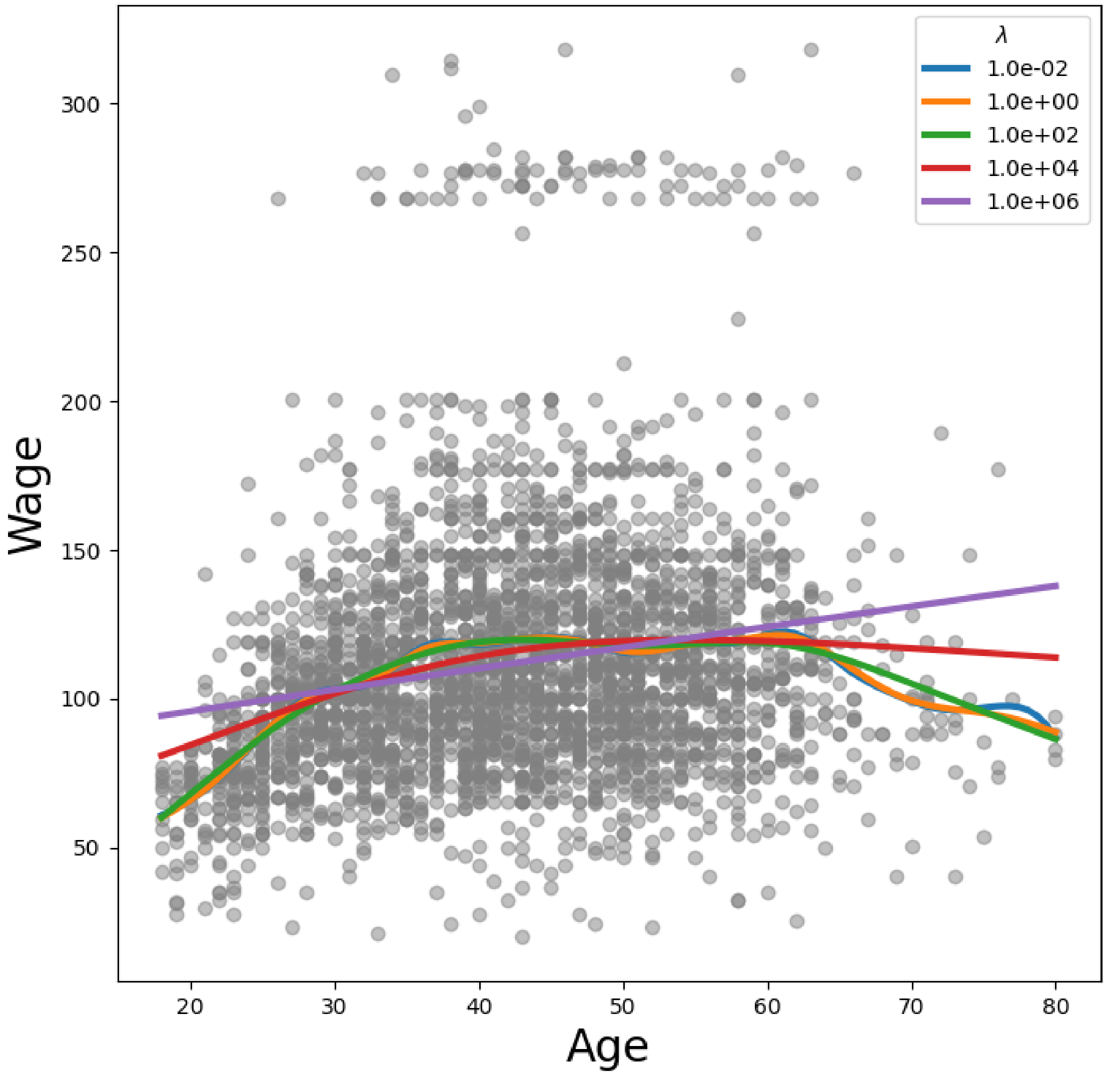
```
gam.fit(X_age, y)
```

[23]:
```
LinearGAM(callbacks=[Deviance(), Diffs()], fit_intercept=True,
   max_iter=100, scale=None, terms=s(0) + intercept, tol=0.0001,
   verbose=False)
```

The pygam library generally expects a matrix of features so we reshape age to be a matrix (a two-dimensional array) instead of a vector (i.e. a onedimensional array). The -1 in the call to the reshape() method tells numpy to impute the size of that dimension based on the remaining entries of the shape tuple

Let's investigate how the ft changes with the smoothing parameter lam. The function np.logspace() is similar to np.linspace() but spaces points evenly on the log-scale. Below we vary lam from 10−2 to 106.

[25]:
```
fig, ax = subplots(figsize=(8,8))
ax.scatter(age, y, facecolor='gray', alpha=0.5)
for lam in np.logspace(-2, 6, 5):
    gam = LinearGAM(s_gam(0, lam=lam)).fit(X_age, y)
    ax.plot(age_grid,gam.predict(age_grid),label='{:.1e}'.
 ↪format(lam),linewidth=3)
ax.set_xlabel('Age', fontsize=20)
ax.set_ylabel('Wage', fontsize=20);
ax.legend(title='$\lambda$');
```

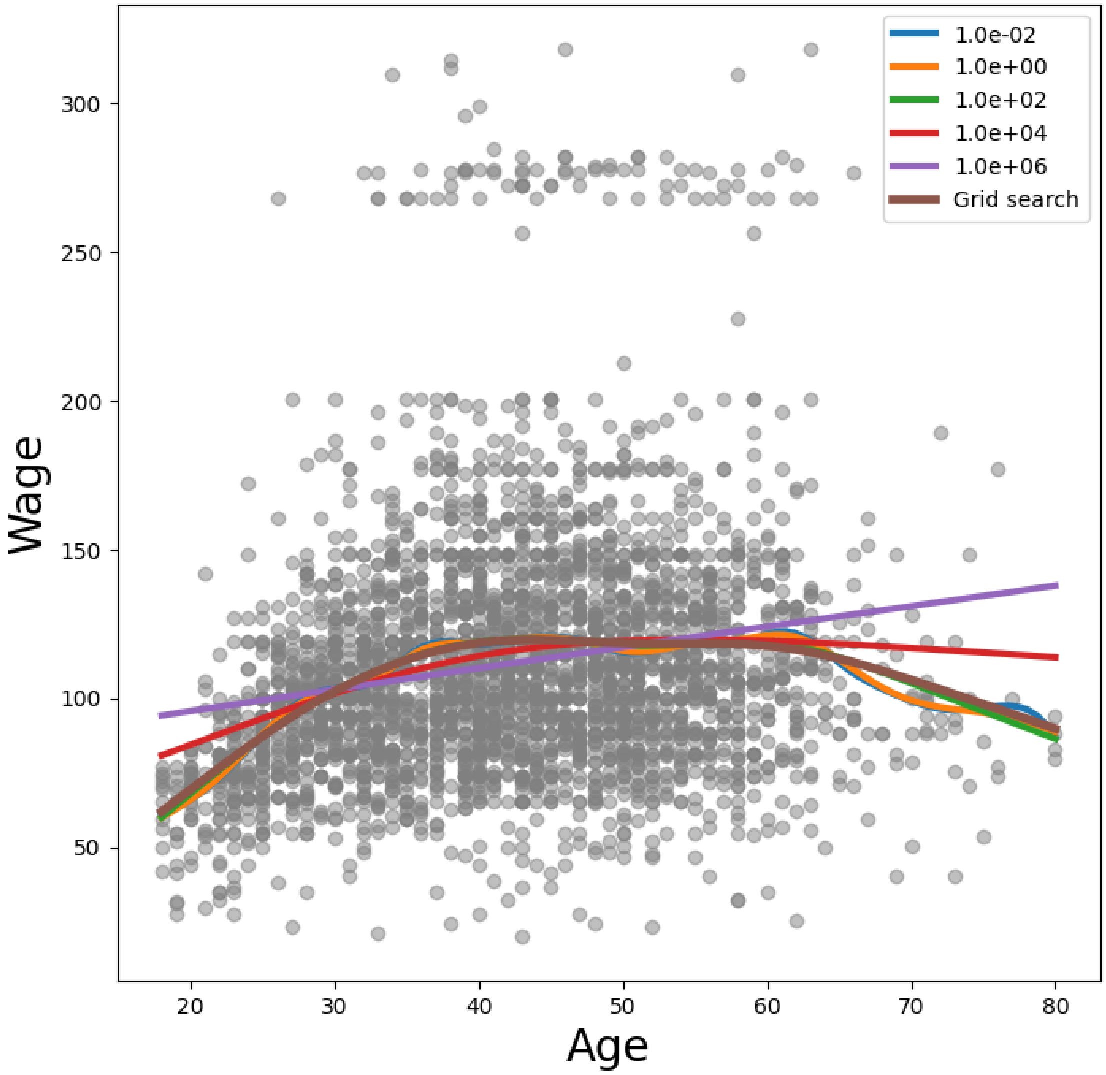


The pygam package can perform a search for an optimal smoothing parameter.

[26]:
```
gam_opt = gam.gridsearch(X_age, y)
ax.plot(age_grid,gam_opt.predict(age_grid),label='Grid search',linewidth=4)
ax.legend()
fig
```

```
100% (11 of 11)
|########################| Elapsed Time: 0:00:00 Time:  0:00:000:00
```

[26]:



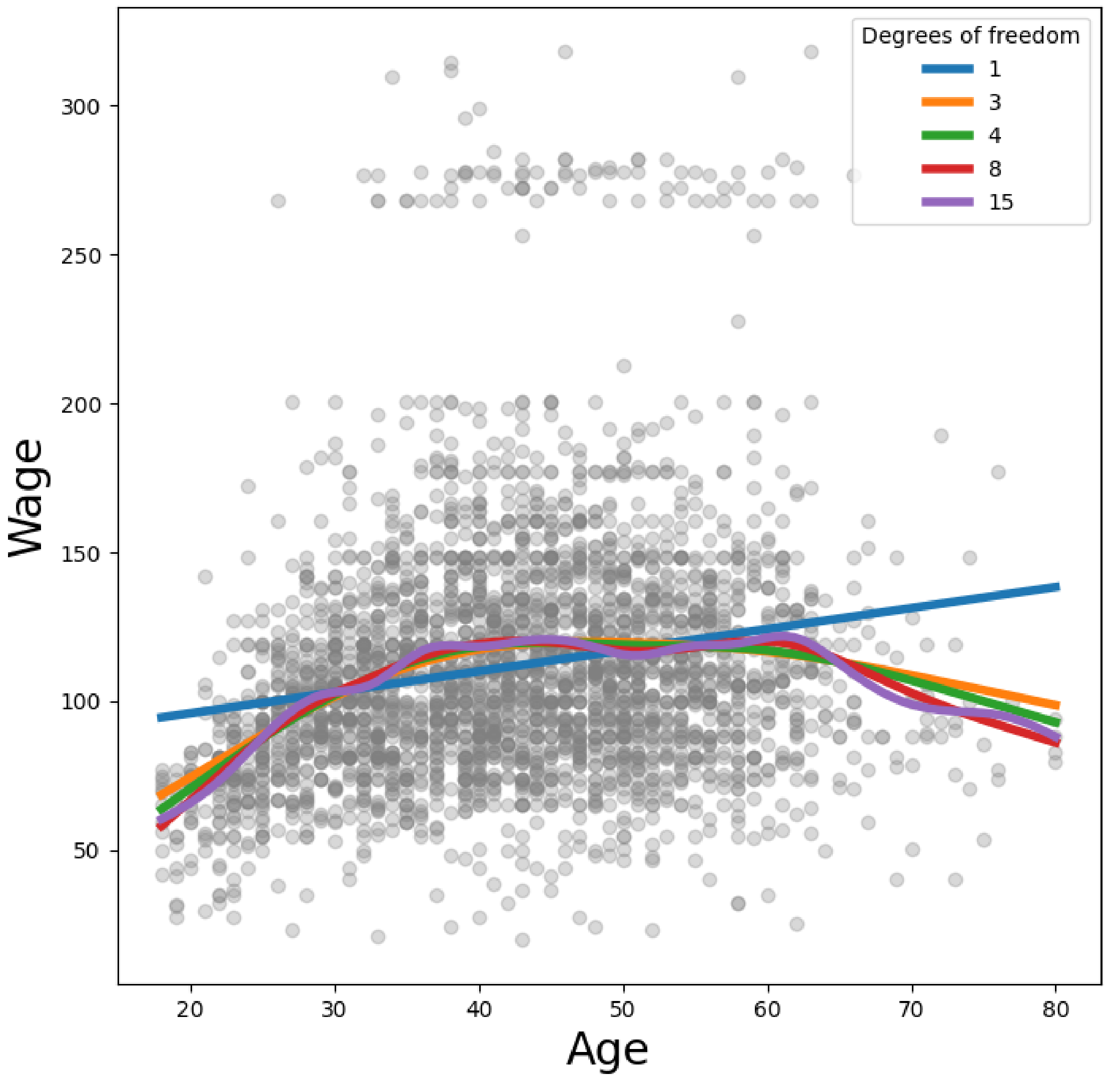
Alternatively, we can fx the degrees of freedom of the smoothing spline using a function included in the ISLP.pygam package. Below we fnd a value of   that gives us roughly four degrees of freedom. We note here that these degrees of freedom include the unpenalized intercept and linear term of the smoothing spline, hence there are at least two degrees of freedom

[27]:
```
age_term = gam.terms[0]
lam_4 = approx_lam(X_age, age_term, 4)
age_term.lam = lam_4
degrees_of_freedom(X_age, age_term)
```

[27]: 4.00000010000072

Let's vary the degrees of freedom in a similar plot to above. We choose the degrees of freedom as the desired degrees of freedom plus one to account for the fact that these smoothing splines always have an intercept term. Hence, a value of one for df is just a linear ft

[28]:
```
fig, ax = subplots(figsize=(8,8))
ax.scatter(X_age,y,facecolor='gray',alpha=0.3)
for df in [1,3,4,8,15]:
    lam = approx_lam(X_age, age_term, df+1)
    age_term.lam = lam
    gam.fit(X_age, y)
    ax.plot(age_grid,
    gam.predict(age_grid),
    label='{:d}'.format(df),linewidth=4)
ax.set_xlabel('Age', fontsize=20)
ax.set_ylabel('Wage', fontsize=20);
ax.legend(title='Degrees of freedom');
```



0.3.1 Additive Models with Several Terms

The strength of generalized additive models lies in their ability to ft multivariate regression models with more fexibility than linear models. We demonstrate two approaches: the frst in a more manual fashion using natural splines and piecewise constant functions, and the second using the pygam package and smoothing splines.

We now ft a GAM by hand to predict wage using natural spline functions of year and age, treating education as a qualitative predictor, as in (7.16). Since this is just a big linear regression model using an appropriate choice of basis functions, we can simply do this using the sm.OLS() function.

We will build the model matrix in a more manual fashion here, since we wish to access the pieces separately when constructing partial dependence plots.

[29]:
```
ns_age = NaturalSpline(df=4).fit(age)
ns_year = NaturalSpline(df=5).fit(Wage['year'])
Xs = [ns_age.transform(age),ns_year.transform(Wage['year']),pd.
 ↪get_dummies(Wage['education']).values]
X_bh = np.hstack(Xs)
gam_bh = sm.OLS(y, X_bh).fit()
```

Here the function NaturalSpline() is the workhorse supporting the ns() helper function. We chose to use all columns of the indicator matrix for the categorical variable education, making an intercept redundant. Finally, we stacked the three component matrices horizontally to form the model matrix X_bh.

We now show how to construct partial dependence plots for each of the terms in our rudimentary GAM. We can do this by hand, given grids for age and year. We simply predict with new X matrices, fxing all but one of the features at a time.

[30]:
```
age_grid = np.linspace(age.min(),age.max(),100)
X_age_bh = X_bh.copy()[:100]
X_age_bh[:] = X_bh[:].mean(0)[None,:]
X_age_bh[:,:4] = ns_age.transform(age_grid)
preds = gam_bh.get_prediction(X_age_bh)
bounds_age = preds.conf_int(alpha=0.05)
partial_age = preds.predicted_mean
center = partial_age.mean()
partial_age -= center
bounds_age -= center
fig, ax = subplots(figsize=(8,8))
ax.plot(age_grid, partial_age, 'b', linewidth=3)
ax.plot(age_grid, bounds_age[:,0], 'r--', linewidth=3)
ax.plot(age_grid, bounds_age[:,1], 'r--', linewidth=3)
ax.set_xlabel('Age')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of age on wage', fontsize=20);
```

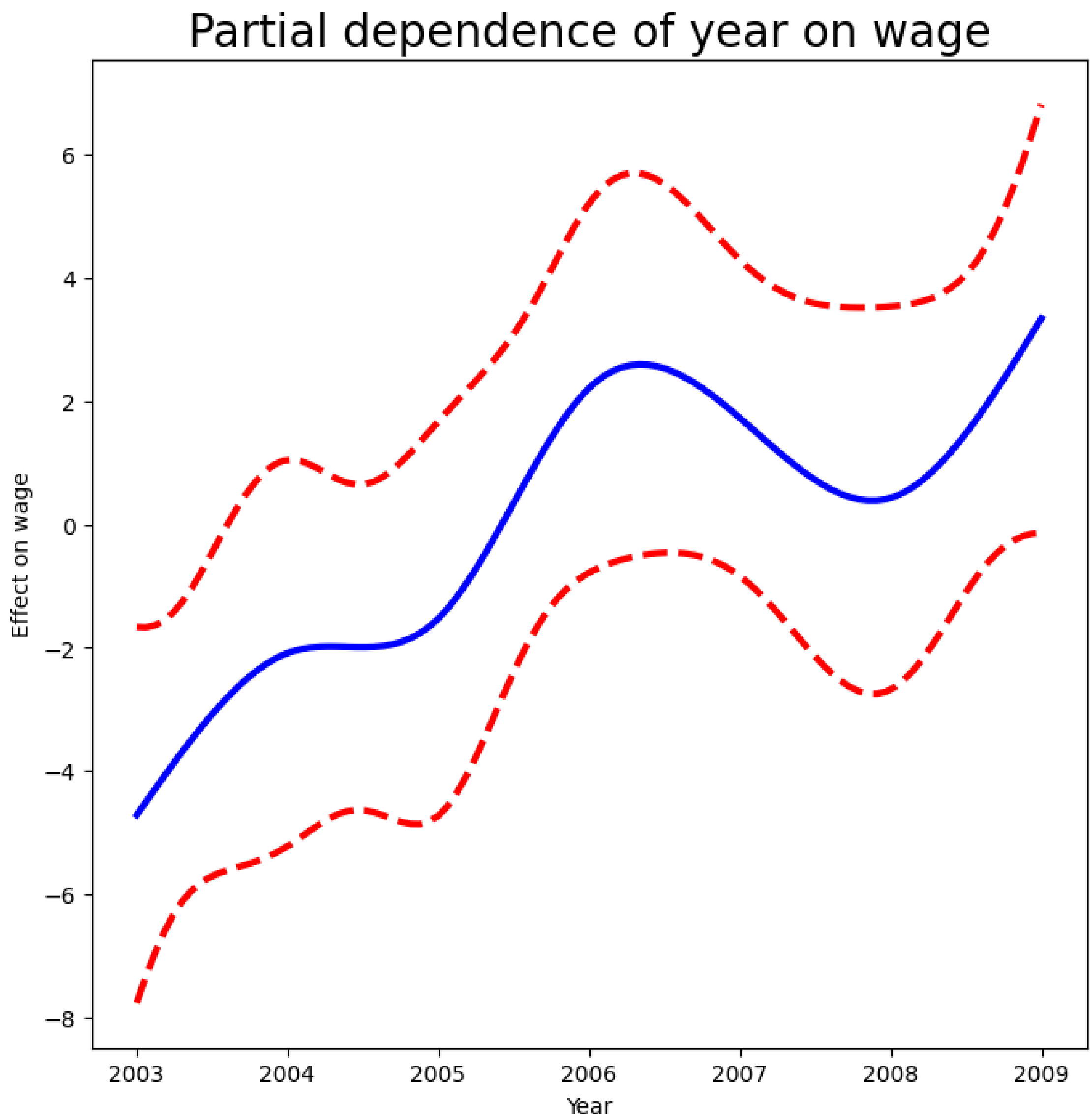
Let's explain in some detail what we did above. The idea is to create a new prediction matrix, where all but the columns belonging to age are constant (and set to their training-data means). The four columns for age are flled in with the natural spline basis evaluated at the 100 values in age_grid.

1. We made a grid of length 100 in age, and created a matrix X_age_bh with 100 rows and the same number of columns as X_bh.
2. We replaced every row of this matrix with the column means of the original.
3. We then replace just the frst four columns representing age with the natural spline basis computed at the values in age_grid.

The remaining steps should by now be familiar.

We also look at the efect of year on wage; the process is the same.

[31]:
```
year_grid = np.linspace(2003, 2009, 100)
year_grid = np.linspace(Wage['year'].min(),Wage['year'].max(),100)
X_year_bh = X_bh.copy()[:100]
X_year_bh[:] = X_bh[:].mean(0)[None,:]
X_year_bh[:,4:9] = ns_year.transform(year_grid)
preds = gam_bh.get_prediction(X_year_bh)
bounds_year = preds.conf_int(alpha=0.05)
partial_year = preds.predicted_mean
center = partial_year.mean()
partial_year -= center
bounds_year -= center
fig, ax = subplots(figsize=(8,8))
ax.plot(year_grid, partial_year , 'b', linewidth=3)
ax.plot(year_grid, bounds_year[:,0], 'r--', linewidth=3)
ax.plot(year_grid, bounds_year[:,1], 'r--', linewidth=3)
ax.set_xlabel('Year')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of year on wage', fontsize=20);
```



We now ft the model (7.16) using smoothing splines rather than natural splines. All of the terms in (7.16) are ft simultaneously, taking each other into account to explain the response. The pygam package only works with matrices, so we must convert the categorical series education to its array representation, which can be found with the cat.codes attribute of education. As year only has 7 unique values, we use only seven basis functions for it

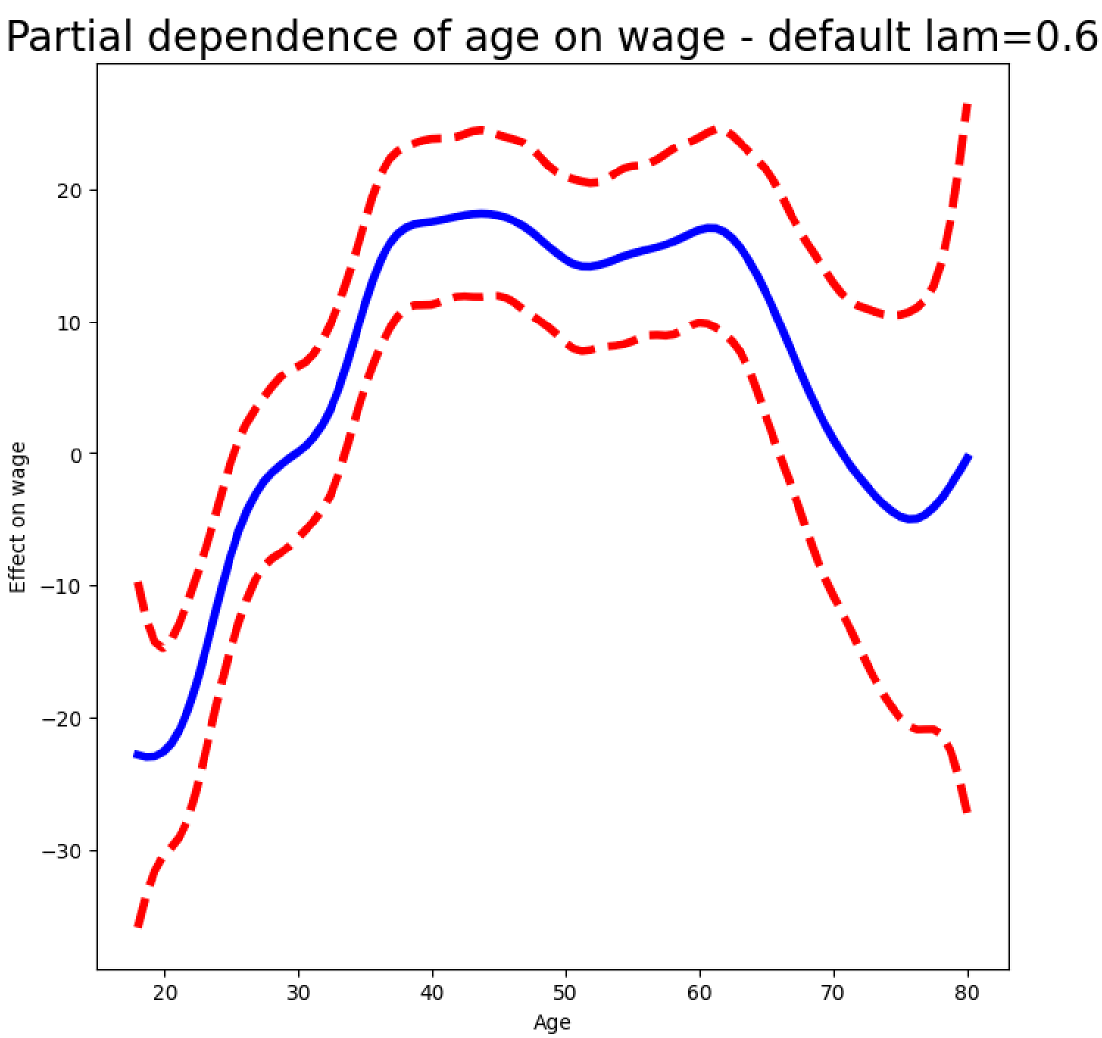
[32]:
```
gam_full = LinearGAM(s_gam(0) +
s_gam(1, n_splines=7) +
f_gam(2, lam=0))
Xgam = np.column_stack([age,
Wage['year'],
Wage['education'].cat.codes])
```

```
gam_full = gam_full.fit(Xgam, y)
```

The two s_gam() terms result in smoothing spline fts, and use a default value for (lam=0.6), which is somewhat arbitrary. For the categorical term education, specifed using a f_gam() term, we specify lam=0 to avoid any shrinkage. We produce the partial dependence plot in age to see the efect of these choices.

The values for the plot are generated by the pygam package. We provide a plot_gam() function for partial-dependence plots in ISLP.pygam, which makes this job easier than in our last example with natural splines.

[33]:
```
fig, ax = subplots(figsize=(8,8))
plot_gam(gam_full, 0, ax=ax)
ax.set_xlabel('Age')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of age on wage - default lam=0.6',fontsize=20);
```



We see that the function is somewhat wiggly. It is more natural to specify the df than a value for lam. We reft a GAM using four degrees of freedom each for age and year. Recall that the addition of one below takes into account the intercept of the smoothing spline.

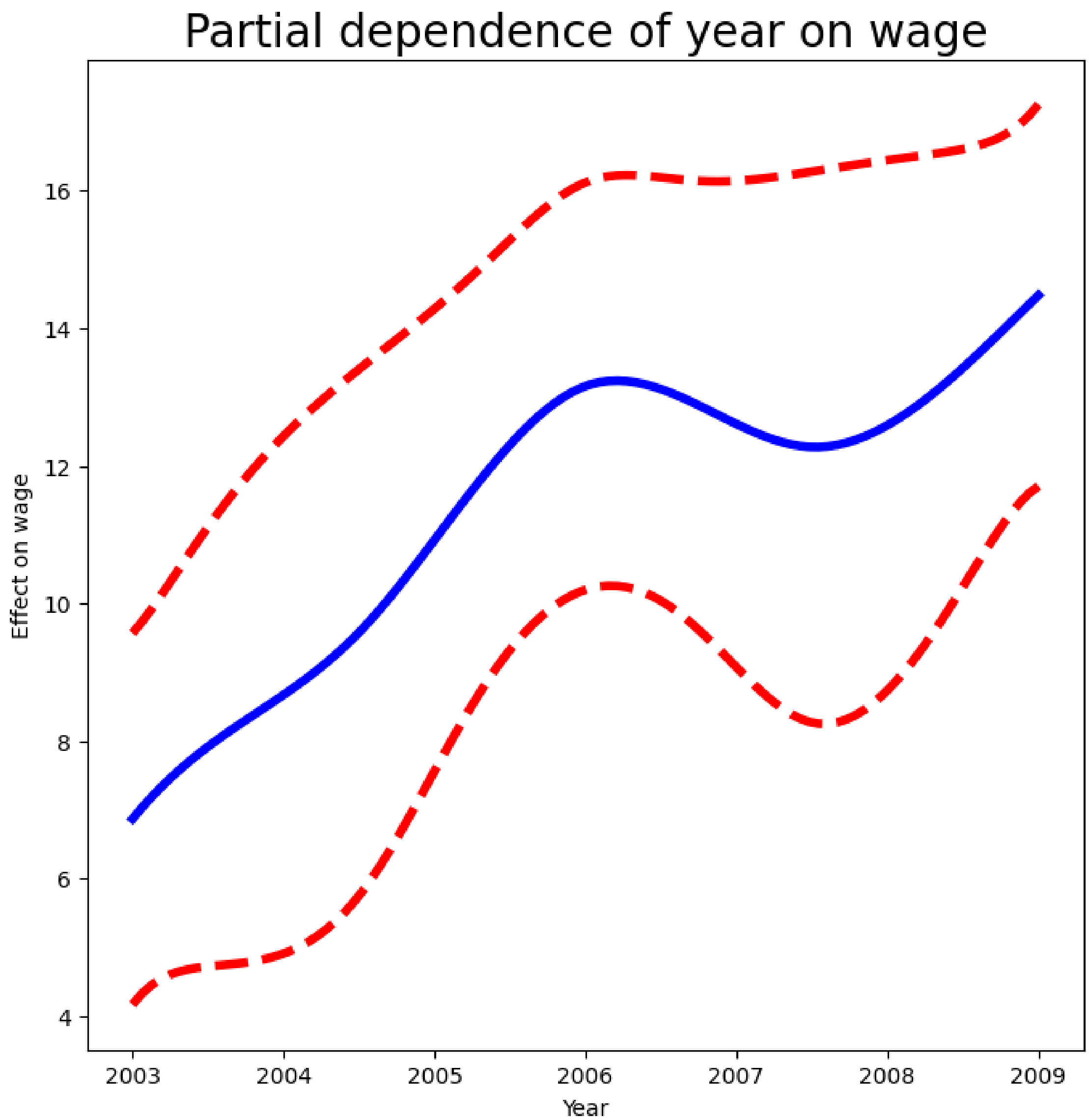
[34]:
```
age_term = gam_full.terms[0]
age_term.lam = approx_lam(Xgam, age_term, df=4+1)
year_term = gam_full.terms[1]
year_term.lam = approx_lam(Xgam, year_term, df=4+1)
gam_full = gam_full.fit(Xgam, y)
```

Note that updating age_term.lam above updates it in gam_full.terms[0] as well! Likewise for year_term.lam.

Repeating the plot for age, we see that it is much smoother. We also produce the plot for year.

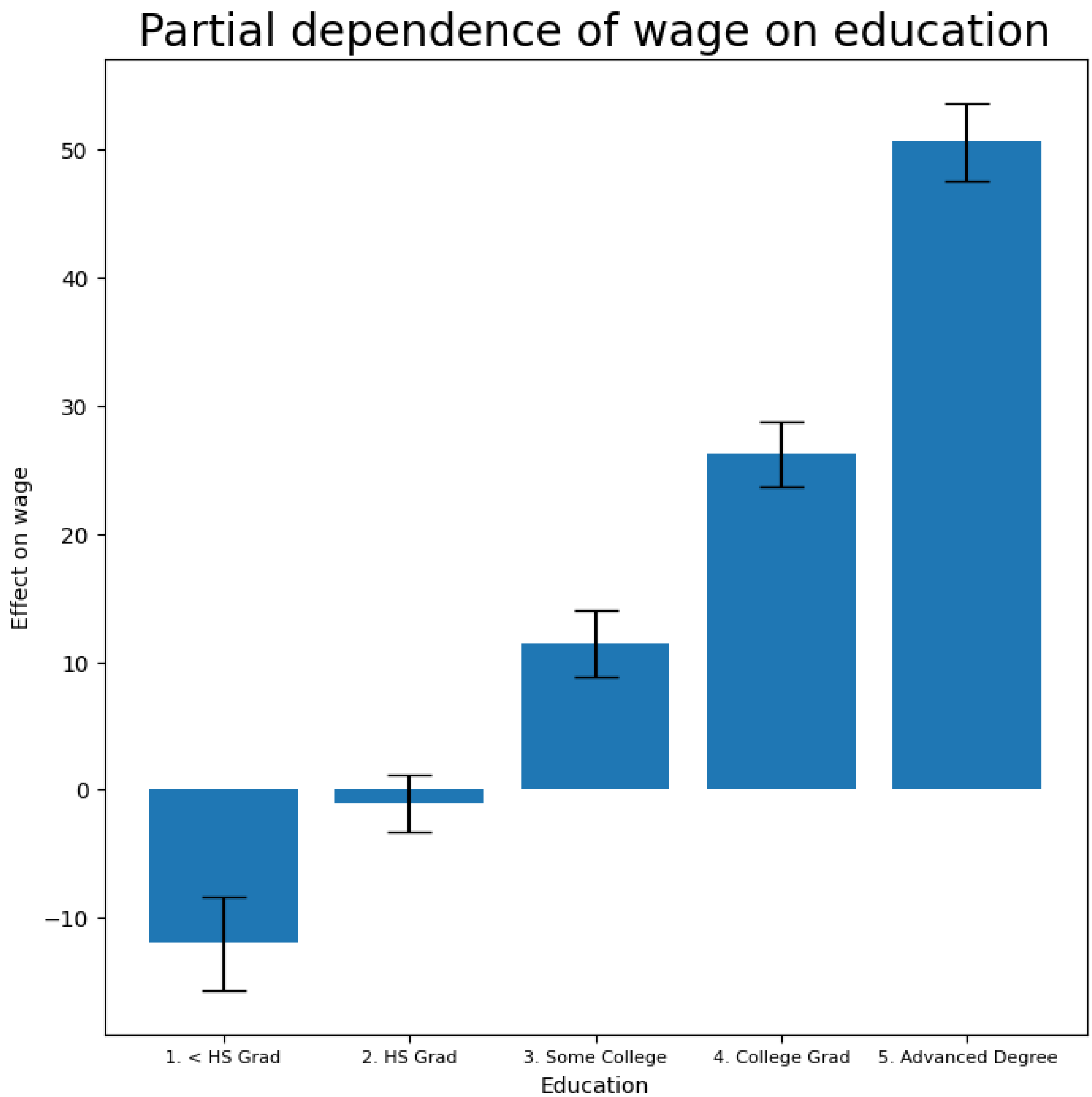
[35]:
```
fig, ax = subplots(figsize=(8,8))
plot_gam(gam_full,1,ax=ax)
ax.set_xlabel('Year')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of year on wage', fontsize=20)
```

[35]:
```
Text(0.5, 1.0, 'Partial dependence of year on wage')
```



Finally we plot education, which is categorical. The partial dependence plot is diferent, and more suitable for the set of ftted constants for each level of this variable.

[36]:
```
fig, ax = subplots(figsize=(8, 8))
ax = plot_gam(gam_full, 2)
ax.set_xlabel('Education')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of wage on education',
fontsize=20);
ax.set_xticklabels(Wage['education'].cat.categories, fontsize=8);
```



0.4 ANOVA Tests for Additive Models

In all of our models, the function of year looks rather linear. We can perform a series of ANOVA tests in order to determine which of these three models is best: a GAM that excludes year (M1), a GAM that uses a linear function of year (M2), or a GAM that uses a spline function of year (M3).

[37]:
```
gam_0 = LinearGAM(age_term + f_gam(2, lam=0))
gam_0.fit(Xgam, y)
gam_linear = LinearGAM(age_term +
l_gam(1, lam=0) +
f_gam(2, lam=0))
gam_linear.fit(Xgam, y)
```

[37]:
```
LinearGAM(callbacks=[Deviance(), Diffs()], fit_intercept=True,
   max_iter=100, scale=None, terms=s(0) + l(1) + f(2) + intercept,
   tol=0.0001, verbose=False)
```

Notice our use of age_term in the expressions above. We do this because earlier we set the value for lam in this term to achieve four degrees of freedom.

To directly assess the efect of year we run an ANOVA on the three models ft above.

[38]:
```
anova_gam(gam_0, gam_linear, gam_full)
```

[38]:

	deviance	df	deviance_diff	df_diff	F	pvalue
0	3.714362e+06	2991.004005	NaN	NaN	NaN	NaN
1	3.696746e+06	2990.005190	17616.542840	0.998815	14.265131	0.002314
2	3.693143e+06	2987.007254	3602.893655	2.997936	0.972007	0.435579

We fnd that there is compelling evidence that a GAM with a linear function in year is better than a GAM that does not include year at all (p-value= 0.002). However, there is no evidence that a non-linear function of year is needed (p-value=0.435). In other words, based on the results of this ANOVA, M2 is preferred.

We can repeat the same process for age as well. We see there is very clear evidence that a non-linear term is required for age.

[39]:
```
gam_0 = LinearGAM(year_term +
f_gam(2, lam=0))
gam_linear = LinearGAM(l_gam(0, lam=0) +
year_term +
f_gam(2, lam=0))
gam_0.fit(Xgam, y)
gam_linear.fit(Xgam, y)
anova_gam(gam_0, gam_linear, gam_full)
```

[39]:

	deviance	df	deviance_diff	df_diff	F	\
0	3.975443e+06	2991.000589	NaN	NaN	NaN	
1	3.850247e+06	2990.000704	125196.137317	0.999884	101.270106	
2	3.693143e+06	2987.007254	157103.978302	2.993450	42.447812	

	pvalue
0	NaN
1	1.681120e-07
2	5.669414e-07

There is a (verbose) summary() method for the GAM ft. (We do not reproduce it here.)

[40]:
```
gam_full.summary()
```

```
LinearGAM
===============================================
==========================================================
Distribution:                      NormalDist Effective DoF:
```

```
12.9927
Link Function:                           IdentityLink Log Likelihood:
-24117.907
Number of Samples:                               3000 AIC:
48263.7995
                                                  AICc:
48263.94
                                                  GCV:
1246.1129
                                                  Scale:
1236.4024
                                                  Pseudo R-Squared:
0.2928
================================================================================
==========================
Feature Function                  Lambda               Rank         EDoF
P > x        Sig. Code
================================= ==================== ============ ============
============ ============
s(0)                              [465.0491]           20           5.1
1.11e-16     ***
s(1)                              [2.1564]             7            4.0
8.10e-03     **
f(2)                              [0]                  5            4.0
1.11e-16     ***
intercept                                              1            0.0
1.11e-16     ***
================================================================================
==========================
Significance codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

WARNING: Fitting splines and a linear function to a feature introduces a model
identifiability problem
         which can cause p-values to appear significant when they are not.

WARNING: p-values calculated in this manner behave correctly for un-penalized
models or models with
         known smoothing parameters, but when smoothing parameters have been
estimated, the p-values
         are typically lower than they should be, meaning that the tests reject
the null too readily.

C:\Users\ankit19.gupta\AppData\Local\Temp\ipykernel_17328\3870570873.py:1:
UserWarning: KNOWN BUG: p-values computed in this summary are likely much
smaller than they should be.

Please do not make inferences based on these values!
```

```
Collaborate on a solution, and stay up to date at:
github.com/dswah/pyGAM/issues/163
```

```
gam_full.summary()
```

We can make predictions from gam objects, just like from lm objects, using the predict() method for the class gam. Here we make predictions on the training set.

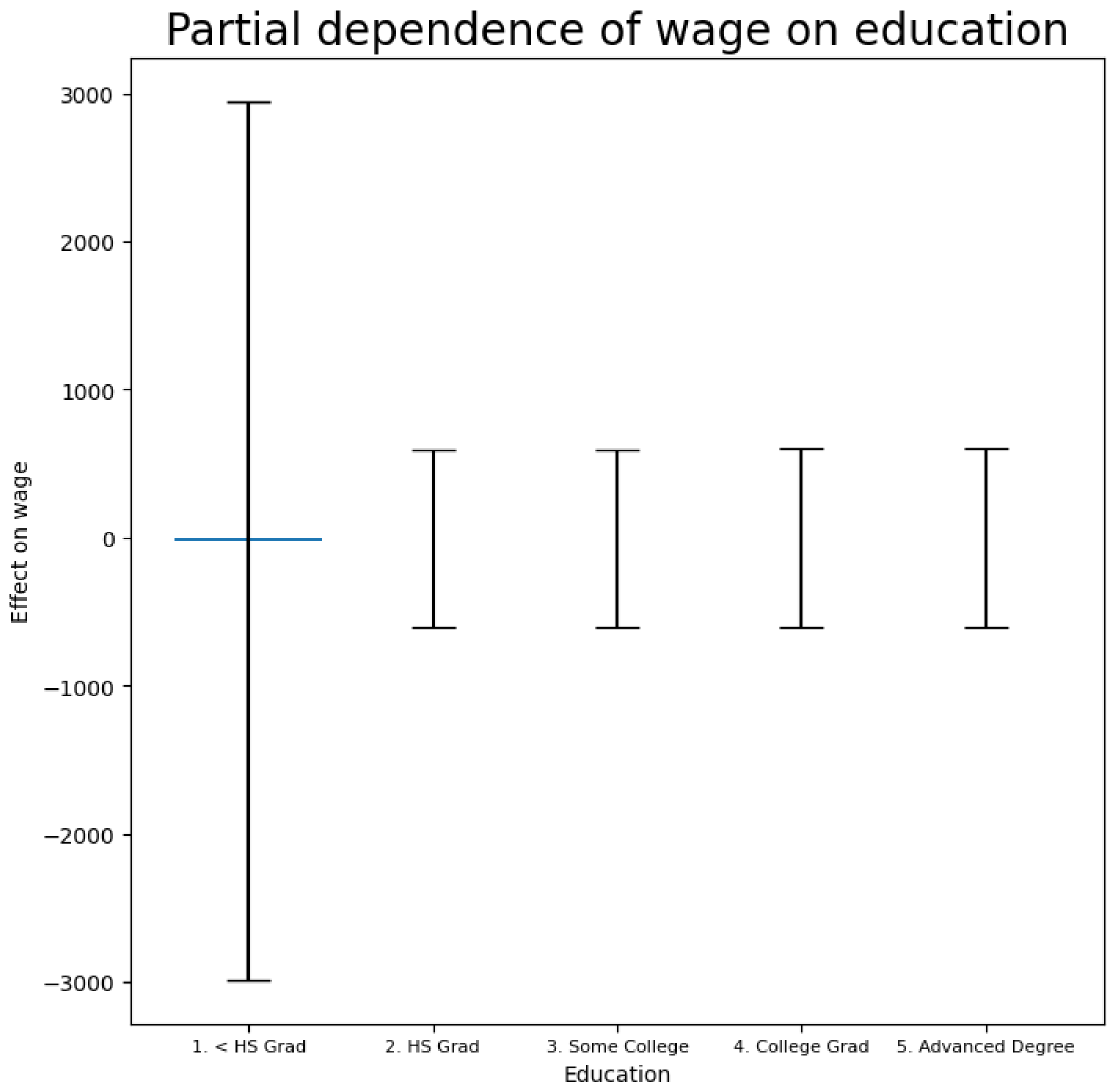
[41]:
```
Yhat = gam_full.predict(Xgam)
```

In order to ft a logistic regression GAM, we use LogisticGAM() from pygam

[42]:
```
gam_logit = LogisticGAM(age_term +
l_gam(1, lam=0) +
f_gam(2, lam=0))
gam_logit.fit(Xgam, high_earn)
```

[42]:
```
LogisticGAM(callbacks=[Deviance(), Diffs(), Accuracy()],
   fit_intercept=True, max_iter=100,
   terms=s(0) + l(1) + f(2) + intercept, tol=0.0001, verbose=False)
```

[43]:
```
fig, ax = subplots(figsize=(8, 8))
ax = plot_gam(gam_logit, 2)
ax.set_xlabel('Education')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of wage on education',
fontsize=20);
ax.set_xticklabels(Wage['education'].cat.categories, fontsize=8);
```



The model seems to be very fat, with especially high error bars for the frst category. Let's look at the data a bit more closely

[44]:
```
pd.crosstab(Wage['high_earn'], Wage['education'])
```

[44]:
```
education  1. < HS Grad  2. HS Grad  3. Some College  4. College Grad  \
high_earn
False               268         966              643              663
True                  0           5                7               22

education  5. Advanced Degree
high_earn
False                     381
True                       45
```

We see that there are no high earners in the frst category of education, meaning that the model will have a hard time ftting. We will ft a logistic regression GAM excluding all observations falling into this category. This provides more sensible results.

To do so, we could subset the model matrix, though this will not remove the column from Xgam. While we can deduce which column corresponds to this feature, for reproducibility's sake we reform the model matrix on this smaller subset.

[46]:
```
only_hs = Wage['education'] == '1. < HS Grad'
Wage_ = Wage.loc[~only_hs]
Xgam_ = np.column_stack([Wage_['age'],
Wage_['year'],
Wage_['education'].cat.codes -1])
high_earn_ = Wage_['high_earn']
```

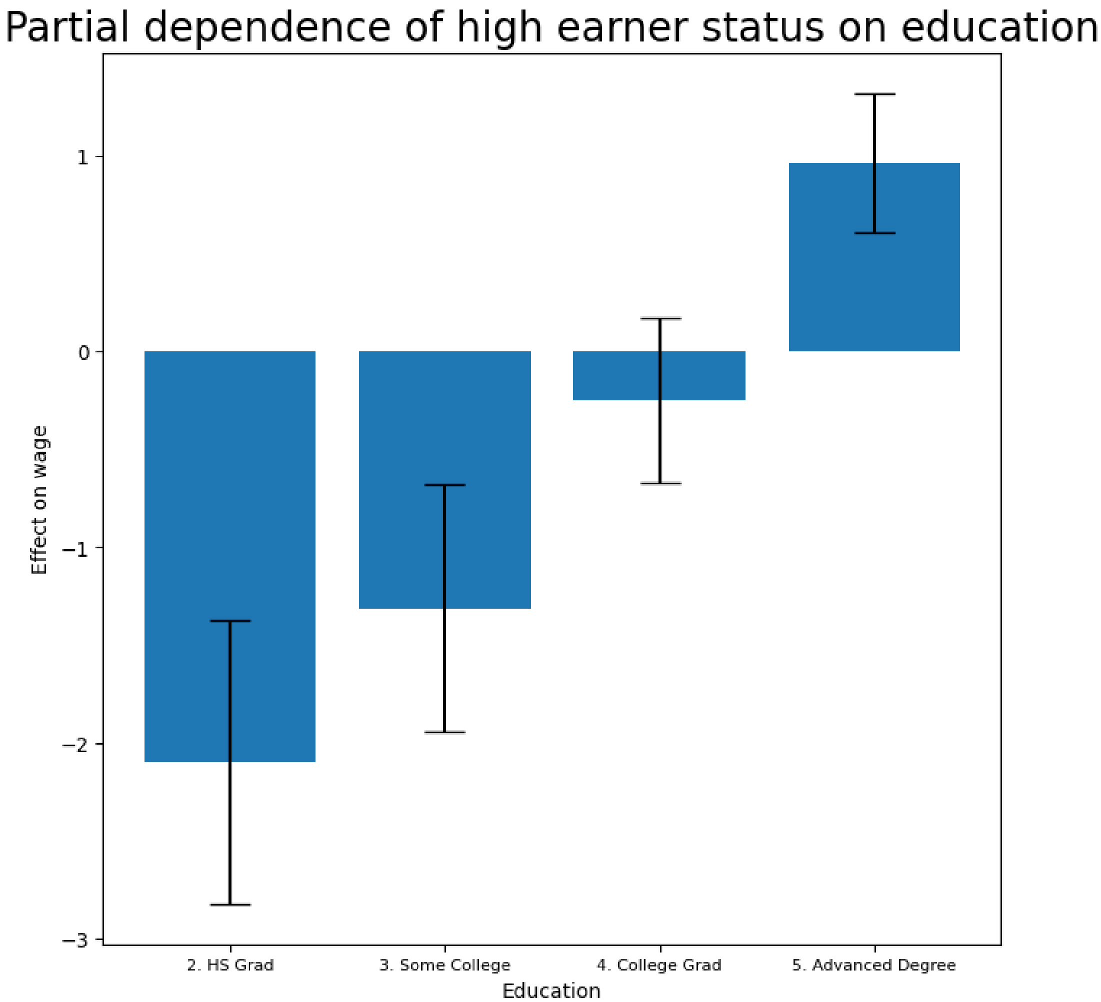
In the second-to-last line above, we subtract one from the codes of the category, due to a bug in pygam. It just relabels the education values and hence has no efect on the ft. We now ft the model.

[47]:
```
gam_logit_ = LogisticGAM(age_term +
year_term +
f_gam(2, lam=0))
gam_logit_.fit(Xgam_, high_earn_)
```

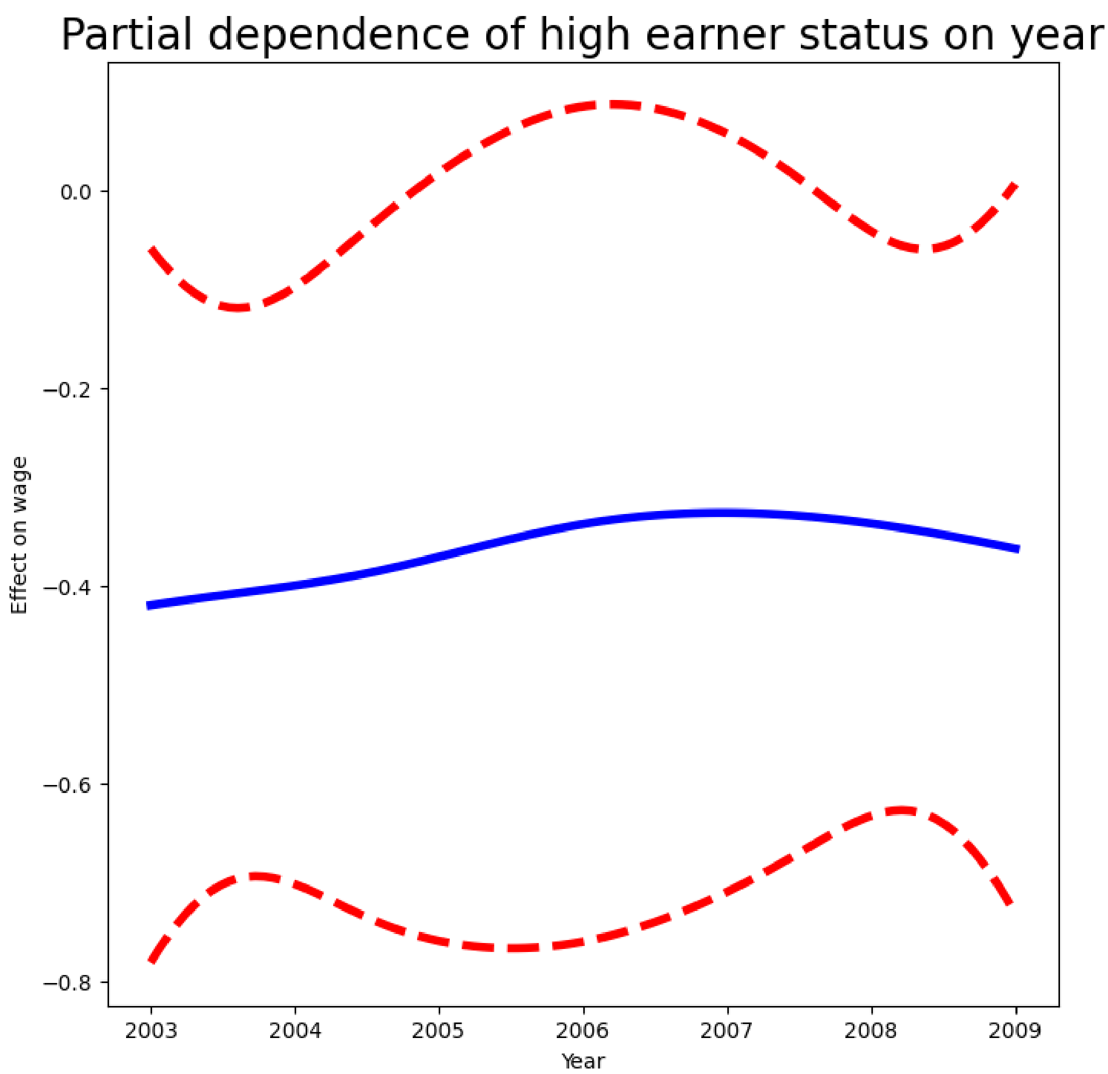
[47]:
```
LogisticGAM(callbacks=[Deviance(), Diffs(), Accuracy()],
   fit_intercept=True, max_iter=100,
   terms=s(0) + s(1) + f(2) + intercept, tol=0.0001, verbose=False)
```

Let's look at the efect of education, year and age on high earner status now that we've removed those observations.

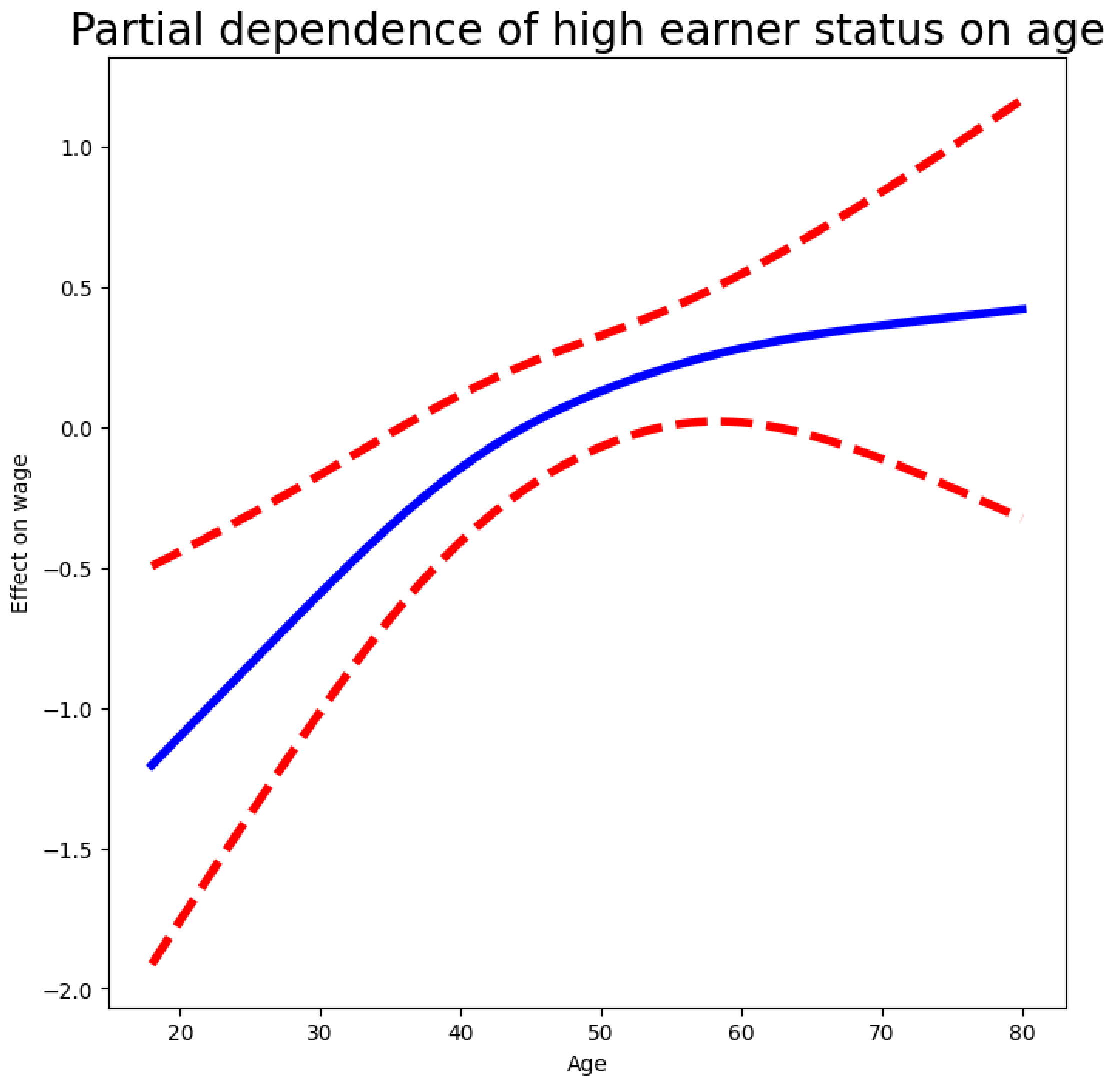
[49]:
```
fig, ax = subplots(figsize=(8, 8))
ax = plot_gam(gam_logit_, 2)
ax.set_xlabel('Education')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of high earner status on education',␣
 ↪fontsize=20);
ax.set_xticklabels(Wage['education'].cat.categories[1:],fontsize=8);
```




```
[51]: fig, ax = subplots(figsize=(8, 8))
      ax = plot_gam(gam_logit_, 1)
      ax.set_xlabel('Year')
      ax.set_ylabel('Effect on wage')
      ax.set_title('Partial dependence of high earner status on year',
      fontsize=20);
```



[52]:
```
fig, ax = subplots(figsize=(8, 8))
ax = plot_gam(gam_logit_, 0)
ax.set_xlabel('Age')
ax.set_ylabel('Effect on wage')
ax.set_title('Partial dependence of high earner status on age',
fontsize=20);
```



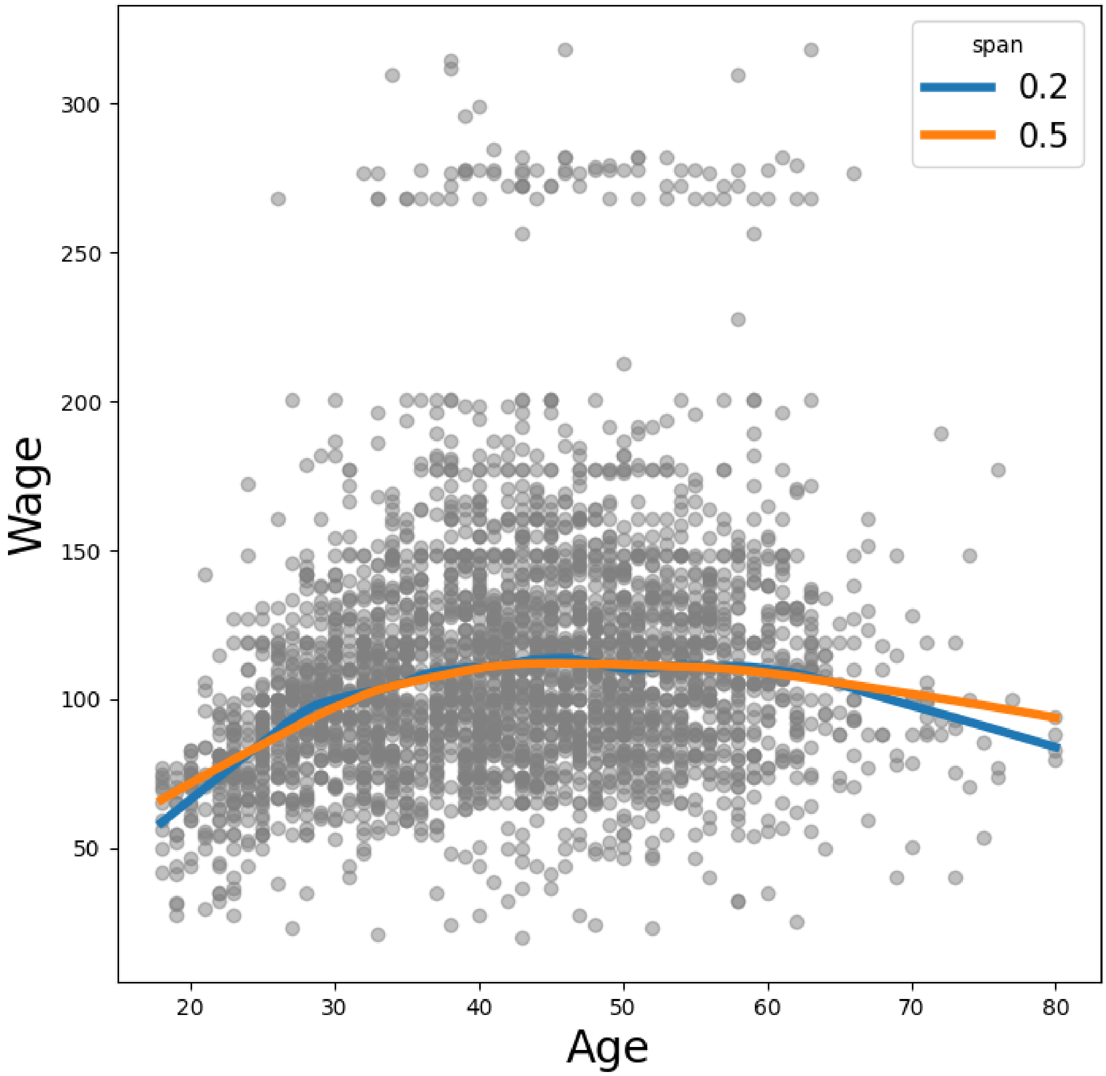
0.5 7.8.4 Local Regression

We illustrate the use of local regression using the lowess() function from sm.nonparametric. Some implementations of GAMs allow terms to be local regression operators; this is not the case in pygam.

Here we ft local linear regression models using spans of 0.2 and 0.5; that is, each neighborhood consists of 20% or 50% of the observations. As expected, using a span of 0.5 is smoother than 0.2.

[54]:
```
lowess = sm.nonparametric.lowess
fig, ax = subplots(figsize=(8,8))
ax.scatter(age, y, facecolor='gray', alpha=0.5)
for span in [0.2, 0.5]:
    fitted = lowess(y,age,frac=span,xvals=age_grid)
```

```
    ax.plot(age_grid,fitted,label='{:.1f}'.format(span),linewidth=4)
ax.set_xlabel('Age', fontsize=20)
ax.set_ylabel('Wage', fontsize=20);
ax.legend(title='span', fontsize=15);
```



[ ]:

```

```