Ch7-nonlin-lab

Lab: Non-linear Modeling

In this lab, we re-analyze the Wage data considered in the examples throughout this chapter, in order to illustrate the fact that many of the complex non-linear fitting procedures discussed can be easily implemented in R. We begin by loading the ISLR2 library, which contains the data.

```
library(ISLR2)
attach(Wage)
```

Polynomial Regression and Step Functions

We now examine how Figure 7.1 was produced. We first fit the model using the following command:

```
fit <- lm(wage ~ poly(age, 4), data = Wage)
coef(summary(fit))</pre>
```

```
## (Intercept) 111.70361 0.7287409 153.283015 0.000000e+00

## poly(age, 4)1 447.06785 39.9147851 11.200558 1.484604e-28

## poly(age, 4)2 -478.31581 39.9147851 -11.983424 2.355831e-32

## poly(age, 4)3 125.52169 39.9147851 3.144742 1.678622e-03

## poly(age, 4)4 -77.91118 39.9147851 -1.951938 5.103865e-02
```

This syntax fits a linear model, using the lm() function, in order to predict wage using a fourth-degree polynomial in age: poly(age, 4). The poly() command allows us to avoid having to write out a long formula with powers of age. The function returns a matrix whose columns are a basis of *orthogonal polynomials*, which essentially means that each column is a linear combination of the variables age, age^2, age^3 and age^4.

However, we can also use poly() to obtain age, age^2, age^3 and age^4 directly, if we prefer. We can do this by using the raw = TRUE argument to the poly() function. Later we see that this does not affect the model in a meaningful way—though the choice of basis clearly affects the coefficient estimates, it does not affect the fitted values obtained.

```
fit2 <- lm(wage ~ poly(age, 4, raw = T), data = Wage)
coef(summary(fit2))</pre>
```

```
## (Intercept) -1.841542e+02 6.004038e+01 -3.067172 0.0021802539

## poly(age, 4, raw = T)1 2.124552e+01 5.886748e+00 3.609042 0.0003123618

## poly(age, 4, raw = T)2 -5.638593e-01 2.061083e-01 -2.735743 0.0062606446

## poly(age, 4, raw = T)3 6.810688e-03 3.065931e-03 2.221409 0.0263977518

## poly(age, 4, raw = T)4 -3.203830e-05 1.641359e-05 -1.951938 0.0510386498
```

There are several other equivalent ways of fitting this model, which showcase the flexibility of the formula language in R. For example

```
## (Intercept) age I(age^2) I(age^3) I(age^4)
## -1.841542e+02 2.124552e+01 -5.638593e-01 6.810688e-03 -3.203830e-05
```

This simply creates the polynomial basis functions on the fly, taking care to protect terms like age^2 via the function I() (the ^ symbol has a special meaning in formulas).

```
fit2b <- lm(wage ~ cbind(age, age^2, age^3, age^4),
    data = Wage)</pre>
```

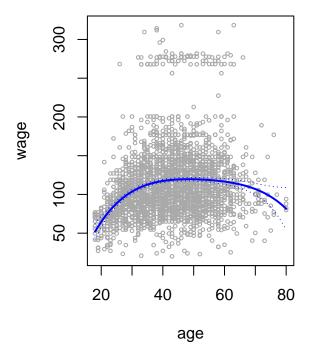
This does the same more compactly, using the cbind() function for building a matrix from a collection of vectors; any function call such as cbind() inside a formula also serves as a wrapper.

We now create a grid of values for age at which we want predictions, and then call the generic predict() function, specifying that we want standard errors as well.

```
agelims <- range(age)
age.grid <- seq(from = agelims[1], to = agelims[2])
preds <- predict(fit, newdata = list(age = age.grid),
    se = TRUE)
se.bands <- cbind(preds$fit + 2 * preds$se.fit,
    preds$fit - 2 * preds$se.fit)</pre>
```

Finally, we plot the data and add the fit from the degree-4 polynomial.

Degree-4 Polynomial



Here the mar and oma arguments to par() allow us to control the margins of the plot, and the title() function creates a figure title that spans both subplots.

We mentioned earlier that whether or not an orthogonal set of basis functions is produced in the poly() function will not affect the model obtained in a meaningful way. What do we mean by this? The fitted values obtained in either case are identical:

```
preds2 <- predict(fit2, newdata = list(age = age.grid),
    se = TRUE)
max(abs(preds$fit - preds2$fit))</pre>
```

[1] 9.353585e-11

In performing a polynomial regression we must decide on the degree of the polynomial to use. One way to do this is by using hypothesis tests. We now fit models ranging from linear to a degree-5 polynomial and seek to determine the simplest model which is sufficient to explain the relationship between wage and age. We use the anova() function, which performs an analysis of variance (ANOVA, using an F-test) in order to test the null hypothesis that a model \mathcal{M}_1 is sufficient to explain the data against the alternative hypothesis that a more complex model \mathcal{M}_2 is required. In order to use the anova() function, \mathcal{M}_1 and \mathcal{M}_2 must be nested models: the predictors in \mathcal{M}_1 must be a subset of the predictors in \mathcal{M}_2 . In this case, we fit five different models and sequentially compare the simpler model to the more complex model.

```
fit.1 <- lm(wage ~ age, data = Wage)
fit.2 <- lm(wage ~ poly(age, 2), data = Wage)
fit.3 <- lm(wage ~ poly(age, 3), data = Wage)
fit.4 <- lm(wage ~ poly(age, 4), data = Wage)</pre>
```

```
fit.5 <- lm(wage ~ poly(age, 5), data = Wage)
anova(fit.1, fit.2, fit.3, fit.4, fit.5)</pre>
```

```
## Analysis of Variance Table
##
## Model 1: wage ~ age
## Model 2: wage ~ poly(age, 2)
## Model 3: wage ~ poly(age, 3)
## Model 4: wage ~ poly(age, 4)
## Model 5: wage ~ poly(age, 5)
     Res.Df
                RSS Df Sum of Sq
                                             Pr(>F)
## 1
       2998 5022216
## 2
       2997 4793430
                          228786 143.5931 < 2.2e-16 ***
## 3
       2996 4777674
                           15756
                                   9.8888 0.001679 **
                     1
## 4
       2995 4771604
                            6070
                                   3.8098
                                           0.051046 .
## 5
       2994 4770322 1
                            1283
                                   0.8050
                                           0.369682
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
```

The p-value comparing the linear Model 1 to the quadratic Model 2 is essentially zero ($<10^{-15}$), indicating that a linear fit is not sufficient. Similarly the p-value comparing the quadratic Model 2 to the cubic Model 3 is very low (0.0017), so the quadratic fit is also insufficient. The p-value comparing the cubic and degree-4 polynomials, Model 3 and Model 4, is approximately 5% while the degree-5 polynomial Model 5 seems unnecessary because its p-value is 0.37. Hence, either a cubic or a quartic polynomial appear to provide a reasonable fit to the data, but lower- or higher-order models are not justified.

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.

```
coef(summary(fit.5))
```

```
##
                   Estimate Std. Error
                                                       Pr(>|t|)
                                           t value
## (Intercept)
                  111.70361 0.7287647 153.2780243 0.000000e+00
## poly(age, 5)1 447.06785 39.9160847 11.2001930 1.491111e-28
## poly(age, 5)2 -478.31581 39.9160847 -11.9830341 2.367734e-32
## poly(age, 5)3
                 125.52169 39.9160847
                                         3.1446392 1.679213e-03
## poly(age, 5)4
                 -77.91118 39.9160847
                                        -1.9518743 5.104623e-02
## poly(age, 5)5 -35.81289 39.9160847
                                        -0.8972045 3.696820e-01
```

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() function; for example:

```
(-11.983)^2
```

```
## [1] 143.5923
```

However, the ANOVA method works whether or not we used orthogonal polynomials; it also works when we have other terms in the model as well. For example, we can use anova() to compare these three models:

```
fit.1 <- lm(wage ~ education + age, data = Wage)
fit.2 <- lm(wage ~ education + poly(age, 2), data = Wage)
fit.3 <- lm(wage ~ education + poly(age, 3), data = Wage)
anova(fit.1, fit.2, fit.3)</pre>
```

```
## Analysis of Variance Table
##
## Model 1: wage ~ education + age
## Model 2: wage ~ education + poly(age, 2)
## Model 3: wage ~ education + poly(age, 3)
                RSS Df Sum of Sq
                                        F Pr(>F)
##
    Res.Df
## 1
       2994 3867992
## 2
       2993 3725395 1
                          142597 114.6969 <2e-16 ***
       2992 3719809 1
                            5587
                                   4.4936 0.0341 *
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
```

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 first we create the appropriate response vector, and then apply the glm() function using family = "binomial" in order to fit a polynomial logistic regression model.

Note that we again use the wrapper I() to create this binary response variable on the fly. The expression wage > 250 evaluates to a logical variable containing TRUEs and FALSEs, which glm() coerces to binary by setting the TRUEs to 1 and the FALSEs to 0.

Once again, we make predictions using the predict() function.

```
preds <- predict(fit, newdata = list(age = age.grid), se = T)</pre>
```

However, calculating the confidence intervals is slightly more involved than in the linear regression case. The default prediction type for a glm() model is type = "link", which is what we use here. This means we get predictions for the logit, or log-odds: that is, we have fit a model of the form

$$\log\left(\frac{\Pr(Y=1|X)}{1-\Pr(Y=1|X)}\right) = X\beta,$$

and the predictions given are of the form $X\hat{\beta}$. The standard errors given are also for $X\hat{\beta}$. In order to obtain confidence intervals for $\Pr(Y=1|X)$, we use the transformation

$$\Pr(Y = 1|X) = \frac{\exp(X\beta)}{1 + \exp(X\beta)}.$$

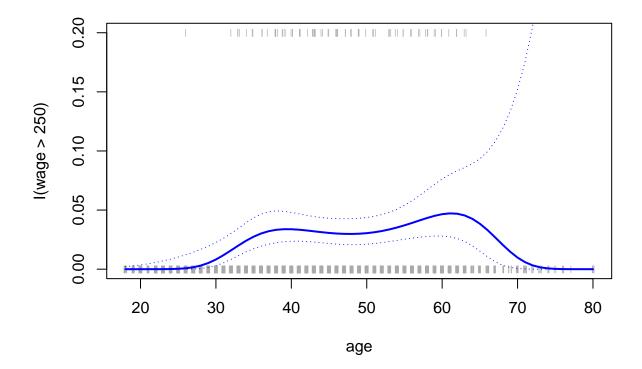
```
pfit <- exp(preds$fit) / (1 + exp(preds$fit))
se.bands.logit <- cbind(preds$fit + 2 * preds$se.fit,
    preds$fit - 2 * preds$se.fit)
se.bands <- exp(se.bands.logit) / (1 + exp(se.bands.logit))</pre>
```

Note that we could have directly computed the probabilities by selecting the type = "response" option in the predict() function.

```
preds <- predict(fit, newdata = list(age = age.grid),
     type = "response", se = T)</pre>
```

However, the corresponding confidence intervals would not have been sensible because we would end up with negative probabilities!

Finally, the right-hand plot from Figure 7.1 was made as follows:



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 used the jitter() function to jitter the age values a bit so that observations with the same age value do not cover each other up. This is often called a .

In order to fit a step function, as discussed in Section 7.2, we use the cut() function.

```
##
## (17.9,33.5] (33.5,49] (49,64.5] (64.5,80.1]
## 750 1399 779 72
```

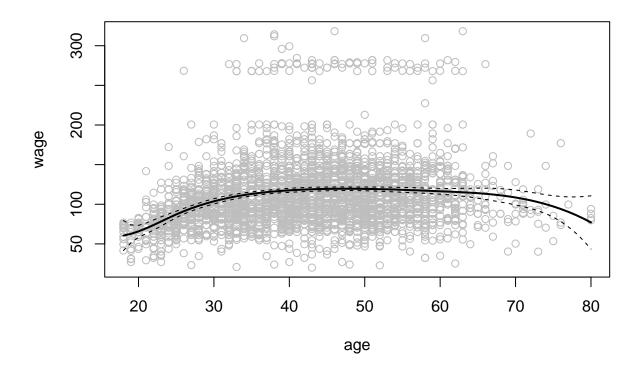
```
fit <- lm(wage ~ cut(age, 4), data = Wage)
coef(summary(fit))</pre>
```

```
## (Intercept) 94.158392 1.476069 63.789970 0.000000e+00
## cut(age, 4)(33.5,49] 24.053491 1.829431 13.148074 1.982315e-38
## cut(age, 4)(49,64.5] 23.664559 2.067958 11.443444 1.040750e-29
## cut(age, 4)(64.5,80.1] 7.640592 4.987424 1.531972 1.256350e-01
```

Here cut() automatically picked the cutpoints at 33.5, 49, and 64.5~years of age. We could also have specified our own cutpoints directly using the breaks option. The function cut() returns an ordered categorical variable; the lm() function then creates a set of dummy variables for use in the regression. The age < 33.5 category is left out, so the intercept coefficient of 94,160 can be interpreted as the average salary for those under 33.5~years of age, and the other coefficients can be interpreted as the average additional salary for those in the other age groups. We can produce predictions and plots just as we did in the case of the polynomial fit.

In order to fit regression splines in R, we use the **splines** library. In Section 7.4, we saw that regression splines can be fit by constructing an appropriate matrix of basis functions. The **bs()** function generates the entire matrix of basis functions for splines with the specified set of knots. By default, cubic splines are produced. Fitting wage to age using a regression spline is simple:

```
library(splines)
fit <- lm(wage ~ bs(age, knots = c(25, 40, 60)), data = Wage)
pred <- predict(fit, newdata = list(age = age.grid), se = T)
plot(age, wage, col = "gray")
lines(age.grid, pred$fit, lwd = 2)
lines(age.grid, pred$fit + 2 * pred$se, lty = "dashed")
lines(age.grid, pred$fit - 2 * pred$se, lty = "dashed")</pre>
```



Here we have prespecified knots at ages 25, 40, and 60. This produces a spline with six basis functions. (Recall that a cubic spline with three knots has seven degrees of freedom; these degrees of freedom are used up by an intercept, plus six basis functions.) We could also use the df option to produce a spline with knots at uniform quantiles of the data.

```
dim(bs(age, knots = c(25, 40, 60)))

## [1] 3000 6

dim(bs(age, df = 6))

## [1] 3000 6

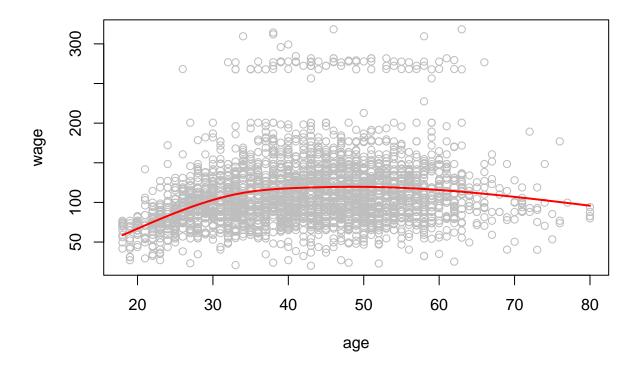
attr(bs(age, df = 6), "knots")

## 25% 50% 75%

## 33.75 42.00 51.00
```

In this case R chooses knots at ages 33.8, 42.0, and 51.0, which correspond to the 25th, 50th, and 75th percentiles of age. The function bs() also has a degree argument, so we can fit splines of any degree, rather than the default degree of 3 (which yields a cubic spline).

In order to instead fit a natural spline, we use the ns() function. Here we fit a natural spline with four degrees of freedom.



As with the bs() function, we could instead specify the knots directly using the knots option.

In order to fit a smoothing spline, we use the **smooth.spline()** function. Figure 7.8 was produced with the following code:

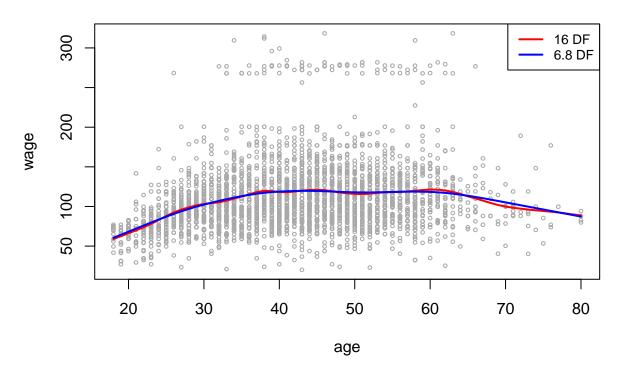
```
plot(age, wage, xlim = agelims, cex = .5, col = "darkgrey")
title("Smoothing Spline")
fit <- smooth.spline(age, wage, df = 16)
fit2 <- smooth.spline(age, wage, cv = TRUE)

## Warning in smooth.spline(age, wage, cv = TRUE): cross-validation with
## non-unique 'x' values seems doubtful</pre>
fit2$df
```

[1] 6.794596

```
lines(fit, col = "red", lwd = 2)
lines(fit2, col = "blue", lwd = 2)
legend("topright", legend = c("16 DF", "6.8 DF"),
    col = c("red", "blue"), lty = 1, lwd = 2, cex = .8)
```

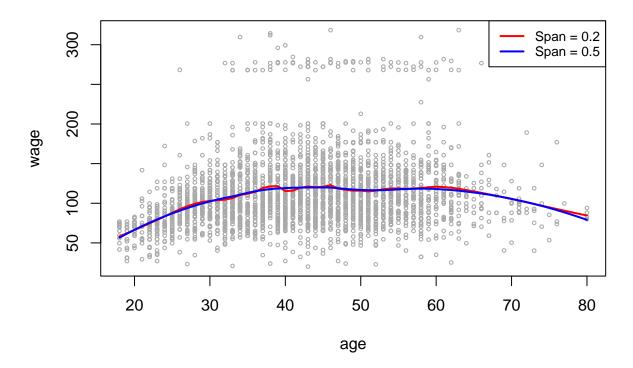
Smoothing Spline



Notice that in the first call to smooth.spline(), we specified df = 16. The function then determines which value of λ leads to 16 degrees of freedom. In the second call to smooth.spline(), we select the smoothness level by cross-validation; this results in a value of λ that yields 6.8 degrees of freedom.

In order to perform local regression, we use the loess() function.

Local Regression



Here we have performed local linear regression using spans of 0.2 and 0.5: that is, each neighborhood consists of 20,% or 50,% of the observations. The larger the span, the smoother the fit. The locfit library can also be used for fitting local regression models in R.

GAMs

We now fit a GAM to predict wage using natural spline functions of lyear 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 lm() function.

```
gam1 <- lm(wage ~ ns(year, 4) + ns(age, 5) + education,
    data = Wage)</pre>
```

We now fit the model (7.16) using smoothing splines rather than natural splines. In order to fit more general sorts of GAMs, using smoothing splines or other components that cannot be expressed in terms of basis functions and then fit using least squares regression, we will need to use the gam library in R.

The s() function, which is part of the gam library, is used to indicate that we would like to use a smoothing spline. We specify that the function of lyear should have 4 degrees of freedom, and that the function of age will have 5 degrees of freedom. Since education is qualitative, we leave it as is, and it is converted into four dummy variables. We use the gam() function in order to fit a GAM using these components. All of the terms in (7.16) are fit simultaneously, taking each other into account to explain the response.

```
library(gam)
```

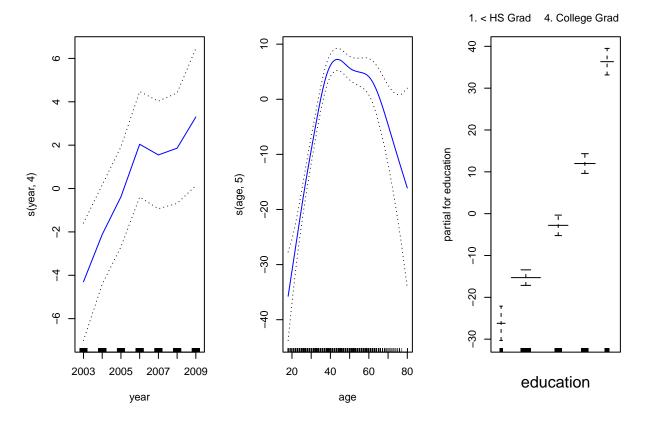
Loading required package: foreach

Loaded gam 1.22-2

```
gam.m3 <- gam(wage ~ s(year, 4) + s(age, 5) + education,
    data = Wage)</pre>
```

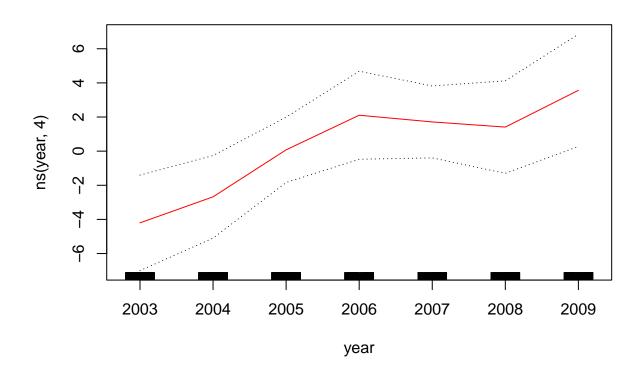
In order to produce Figure 7.12, we simply call the plot() function:

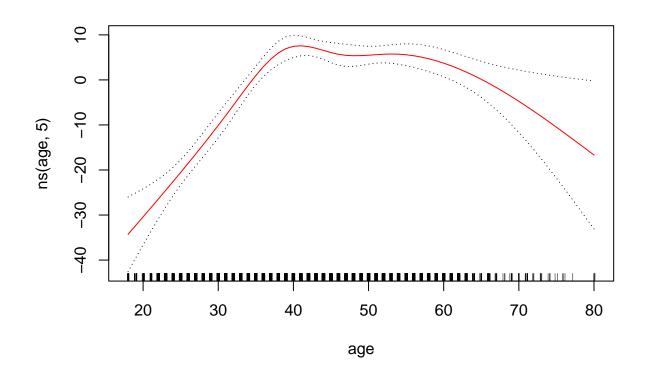
```
par(mfrow = c(1, 3))
plot(gam.m3, se = TRUE, col = "blue")
```

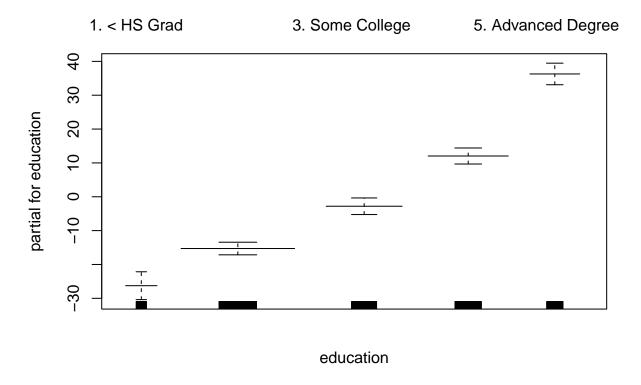


The generic plot() function recognizes that gam.m3 is an object of class Gam, and invokes the appropriate plot.Gam() method. Conveniently, even though gam1 is not of class Gam but rather of class lm, we can still use plot.Gam() on it. Figure 7.11 was produced using the following expression:

```
plot.Gam(gam1, se = TRUE, col = "red")
```







Notice here we had to use plot. Gam() rather than the generic plot() function.

In these plots, the function of lyear 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 lyear (\mathcal{M}_1) , a GAM that uses a linear function of lyear (\mathcal{M}_2) , or a GAM that uses a spline function of lyear (\mathcal{M}_3) .

```
## Analysis of Deviance Table
##
## Model 1: wage ~ s(age, 5) + education
## Model 2: wage ~ year + s(age, 5) + education
## Model 3: wage ~ s(year, 4) + s(age, 5) + education
##
     Resid. Df Resid. Dev Df Deviance
                                                  Pr(>F)
                                             F
## 1
          2990
                  3711731
## 2
          2989
                  3693842
                               17889.2 14.4771 0.0001447 ***
                            1
## 3
          2986
                  3689770
                           3
                                4071.1 1.0982 0.3485661
##
                     '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
```

We find that there is compelling evidence that a GAM with a linear function of lyear is better than a GAM that does not include lyear at all (p-value = 0.00014). However, there is no evidence that a non-linear function of lyear is needed (p-value,=,0.349). In other words, based on the results of this ANOVA, \mathcal{M}_2 is preferred.

The summary() function produces a summary of the gam fit.

```
summary(gam.m3)
```

```
##
## Call: gam(formula = wage ~ s(year, 4) + s(age, 5) + education, data = Wage)
## Deviance Residuals:
##
                1Q Median
                                3Q
      Min
                                       Max
## -119.43
           -19.70
                    -3.33
                             14.17
                                    213.48
##
  (Dispersion Parameter for gaussian family taken to be 1235.69)
##
##
       Null Deviance: 5222086 on 2999 degrees of freedom
##
## Residual Deviance: 3689770 on 2986 degrees of freedom
## AIC: 29887.75
##
## Number of Local Scoring Iterations: NA
##
## Anova for Parametric Effects
##
               Df
                   Sum Sq Mean Sq F value
                     27162
                            27162 21.981 2.877e-06 ***
## s(year, 4)
                1 195338 195338 158.081 < 2.2e-16 ***
## s(age, 5)
                           267432 216.423 < 2.2e-16 ***
## education
                4 1069726
## Residuals 2986 3689770
                              1236
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## Anova for Nonparametric Effects
##
               Npar Df Npar F Pr(F)
## (Intercept)
## s(year, 4)
                     3 1.086 0.3537
## s(age, 5)
                     4 32.380 <2e-16 ***
## education
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

The Anova for Parametric Effects" p-values clearly demonstrate that 'year', 'age', and 'education' are all highly statistically significant, even when only assuming a linear relationship. Alternatively, the Anova for Nonparametric Effects" p-values for year and age correspond to a null hypothesis of a linear relationship versus the alternative of a non-linear relationship. The large p-value for year reinforces our conclusion from the ANOVA test that a linear function is adequate for this term. However, there is very clear evidence that a non-linear term is required for age.

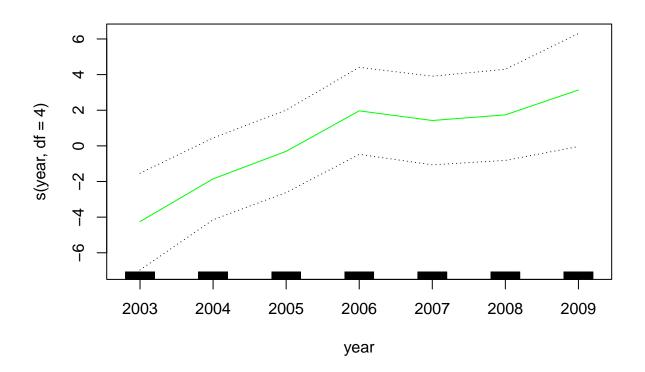
We can make predictions using the predict() method for the class Gam. Here we make predictions on the training set.

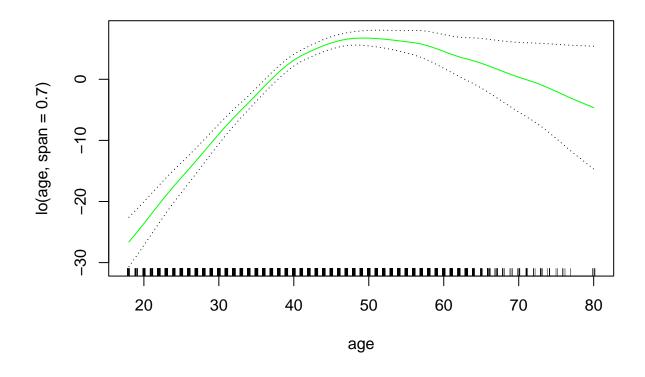
```
preds <- predict(gam.m2, newdata = Wage)</pre>
```

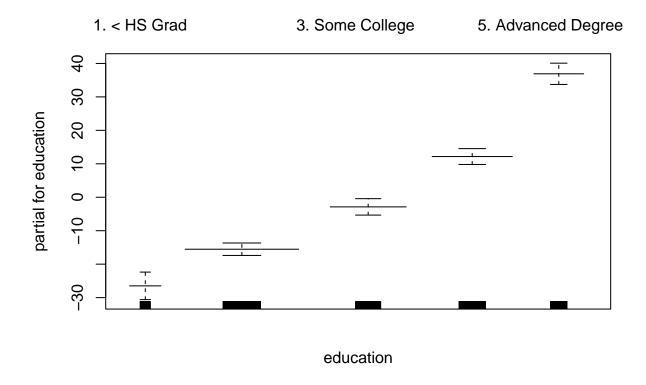
We can also use local regression fits as building blocks in a GAM, using the lo() function.

```
gam.lo <- gam(
   wage ~ s(year, df = 4) + lo(age, span = 0.7) + education,
   data = Wage</pre>
```

```
plot.Gam(gam.lo, se = TRUE, col = "green")
```



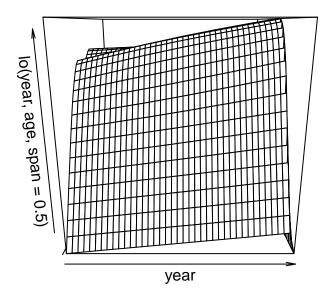


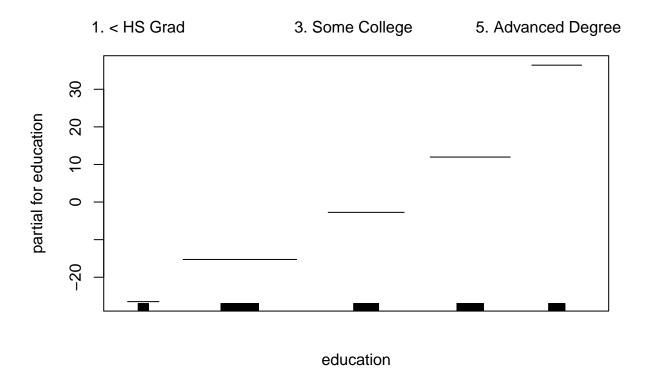


Here we have used local regression for the age term, with a span of 0.7. We can also use the lo() function to create interactions before calling the gam() function. For example,

fits a two-term model, in which the first term is an interaction between lyear and age, fit by a local regression surface. We can plot the resulting two-dimensional surface if we first install the akima package.

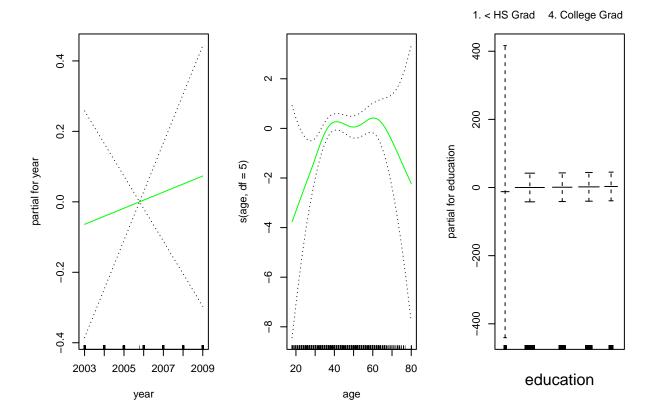
```
library(akima)
plot(gam.lo.i)
```





In order to fit a logistic regression GAM, we once again use the I() function in constructing the binary response variable, and set family=binomial.

```
gam.lr <- gam(
    I(wage > 250) ~ year + s(age, df = 5) + education,
    family = binomial, data = Wage
)
par(mfrow = c(1, 3))
plot(gam.lr, se = T, col = "green")
```



It is easy to see that there are no high earners in the < HS category:

```
table(education, I(wage > 250))
```

```
##
## education
                          FALSE TRUE
##
     1. < HS Grad
                            268
                                   0
                                   5
     2. HS Grad
                            966
##
##
     3. Some College
                            643
                                   7
     4. College Grad
                            663
                                  22
##
     5. Advanced Degree
                            381
                                  45
```

Hence, we fit a logistic regression GAM using all but this category. This provides more sensible results.

```
gam.lr.s <- gam(
    I(wage > 250) ~ year + s(age, df = 5) + education,
    family = binomial, data = Wage,
    subset = (education != "1. < HS Grad")
)
plot(gam.lr.s, se = T, col = "green")</pre>
```

