Moving Beyond Linearity

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Contents

Introduction

Here we explore the use of nonlinear models using some tools in R

```
library(ISLR)
attach(Wage)
```

Polynomials

First we will use polynomials, and focus on a single predictor age:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + ... + \beta_d x_i^d + \epsilon_i$$

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

```
##
## Call:
## lm(formula = wage ~ poly(age, 4), data = Wage)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -98.707 -24.626  -4.993  15.217 203.693
##
## Coefficients:
##                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)    111.7036     0.7287 153.283  < 2e-16 ***
## poly(age, 4)1  447.0679    39.9148  11.201  < 2e-16 ***
## poly(age, 4)2 -478.3158    39.9148 -11.983  < 2e-16 ***
## poly(age, 4)3  125.5217    39.9148   3.145  0.00168 **
## poly(age, 4)4  -77.9112    39.9148  -1.952  0.05104 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 39.91 on 2995 degrees of freedom
## Multiple R-squared:  0.08626,    Adjusted R-squared:  0.08504
## F-statistic: 70.69 on 4 and 2995 DF,  p-value: < 2.2e-16
```

The `poly()` function generates a basis of *orthogonal polynomials* of the 4th order

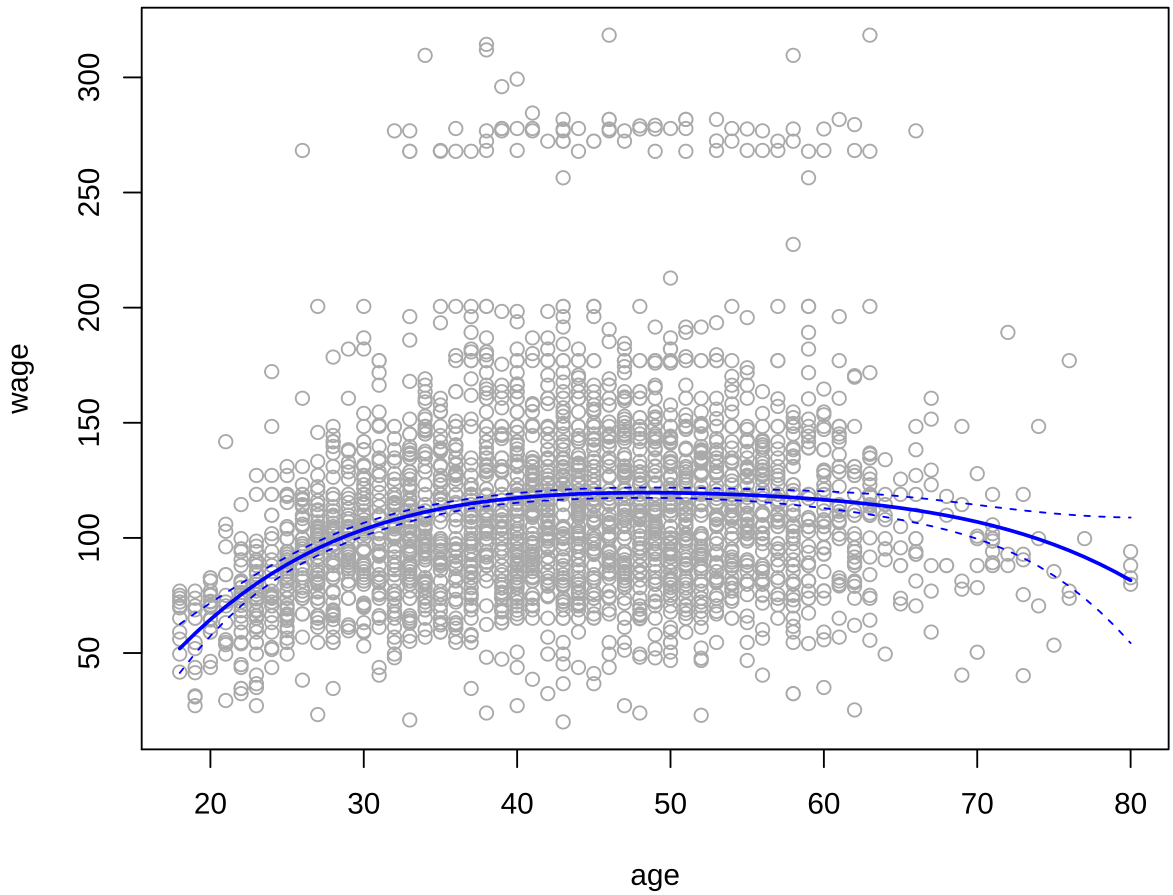
$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_0 + \hat{\beta}_2 x_0^2 + \hat{\beta}_3 x_0^3 + \hat{\beta}_4 x_0^4$$

Lets make a plot of the fitted function, along with the standard errors of the fit.

```
 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, preds$fit-2*preds$se)

plot(age, wage, col="darkgrey")
lines(age.grid, preds$fit, lwd=2, col="blue")
matlines(age.grid, se.bands, col="blue", lty=2)
```



There are other more direct ways of doing this. For example

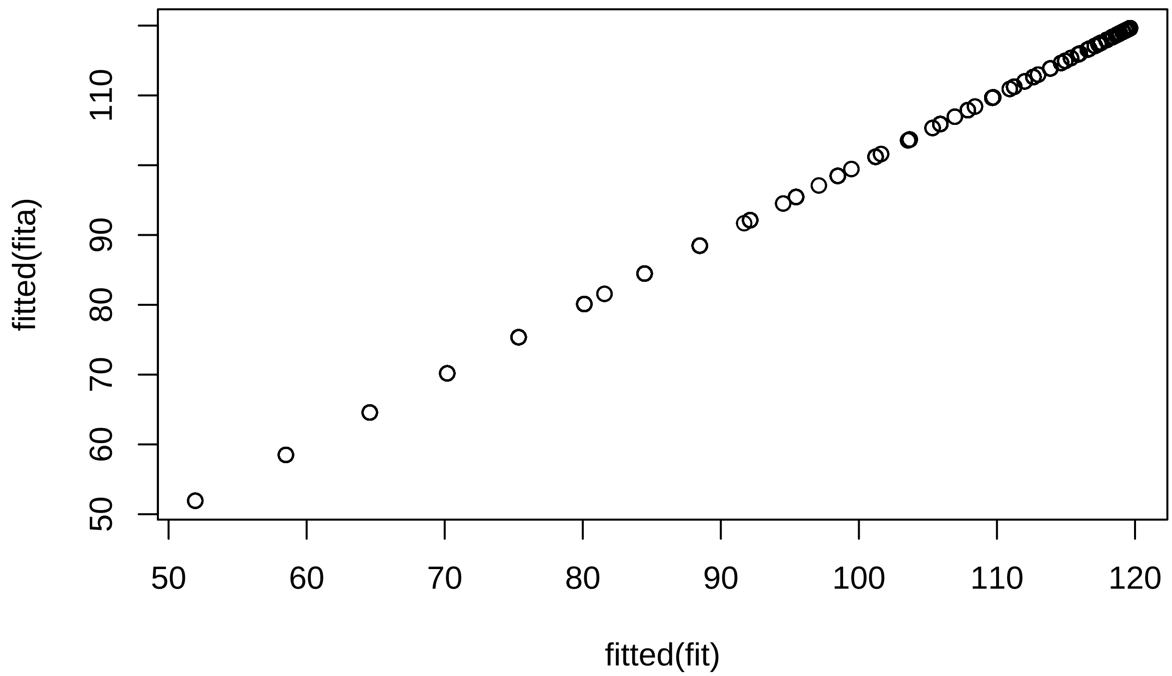
```
fita <- lm(wage~age+I(age^2)+I(age^3)+I(age^4), data = Wage)
summary(fita)
```

```
##
## Call:
## lm(formula = wage ~ age + I(age^2) + I(age^3) + I(age^4), data = Wage)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -98.707 -24.626  -4.993  15.217 203.693
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.842e+02  6.004e+01  -3.067 0.002180 **
## age          2.125e+01  5.887e+00   3.609 0.000312 ***
## I(age^2)    -5.639e-01  2.061e-01  -2.736 0.006261 **
## I(age^3)     6.811e-03  3.066e-03   2.221 0.026398 *
## I(age^4)    -3.204e-05  1.641e-05  -1.952 0.051039 .
```

```
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 39.91 on 2995 degrees of freedom
## Multiple R-squared:  0.08626,    Adjusted R-squared:  0.08504
## F-statistic: 70.69 on 4 and 2995 DF,  p-value: < 2.2e-16
```

Here `I()` is a *wrapper* function; we need it because `age^2` means something to the formula language, while `I(age^2)` is protected. The coefficients are different to those we got before! However, the fits are the same:

```
plot(fitted(fit), fitted(fita))
```



By using orthogonal polynomials in this simple way, it turns out that we can separately test for each coefficient. So if we look at the summary again, we can see that the linear, quadratic and cubic terms are significant, but not the quartic.

```
summary(fit)
```

```
##
## Call:
## lm(formula = wage ~ poly(age, 4), data = Wage)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -98.707 -24.626  -4.993  15.217 203.693
##
## Coefficients:
##                 Estimate Std. Error t value Pr(>|t|)
```

```
## (Intercept)    111.7036     0.7287 153.283  < 2e-16 ***
## poly(age, 4)1  447.0679    39.9148  11.201  < 2e-16 ***
## poly(age, 4)2 -478.3158    39.9148 -11.983  < 2e-16 ***
## poly(age, 4)3  125.5217    39.9148   3.145  0.00168 **
## poly(age, 4)4  -77.9112    39.9148  -1.952  0.05104 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 39.91 on 2995 degrees of freedom
## Multiple R-squared:  0.08626,    Adjusted R-squared:  0.08504
## F-statistic: 70.69 on 4 and 2995 DF,  p-value: < 2.2e-16
```

This only works with linear regression, and if there is a single predictor. In general we would use `anova()` as this next example demonstrates.

```r
fita <- lm(wage ~ education, data = Wage)
fitb <- lm(wage ~ education + age, data = Wage)
fitc <- lm(wage ~ education + poly(age,2), data = Wage)
fitd <- lm(wage ~ education + poly(age,3), data = Wage)

anova(fita, fitb, fitc, fitd)
```

```
## Analysis of Variance Table
##
## Model 1: wage ~ education
## Model 2: wage ~ education + age
## Model 3: wage ~ education + poly(age, 2)
## Model 4: wage ~ education + poly(age, 3)
##   Res.Df     RSS Df Sum of Sq        F Pr(>F)
## 1   2995 3995721
## 2   2994 3867992  1    127729 102.7378 <2e-16 ***
## 3   2993 3725395  1    142597 114.6969 <2e-16 ***
## 4   2992 3719809  1      5587   4.4936 0.0341 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Polynomial logistic regression

Now we fit a logistic regression model to a binary response variable, constructed from `wage`. We code the big earners (`>250K`) as 1, else 0.

$$Pr(y_i > 250|x_i = \frac{exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + ... + \beta_d x_i^d)}{1 + exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + ... + \beta_d x_i^d)}$$

```
fit <- glm(I(wage > 250) ~ poly(age, 3), data = Wage, family = binomial)
summary(fit)
```

```
##
## Call:
## glm(formula = I(wage > 250) ~ poly(age, 3), family = binomial,
##     data = Wage)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -0.2808  -0.2736  -0.2487  -0.1758   3.2868
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept)    -3.8486     0.1597 -24.100  < 2e-16 ***
## poly(age, 3)1  37.8846    11.4818   3.300 0.000968 ***
## poly(age, 3)2 -29.5129    10.5626  -2.794 0.005205 **
## poly(age, 3)3   9.7966     8.9990   1.089 0.276317
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 730.53  on 2999  degrees of freedom
## Residual deviance: 707.92  on 2996  degrees of freedom
## AIC: 715.92
##
## Number of Fisher Scoring iterations: 8
```

```
preds <- predict(fit, list(age = age.grid), se = T)
se.bands <- preds$fit + cbind(fit=0, lower=-2*preds$se, upper=2*preds$se)
se.bands[1:5, ]
```

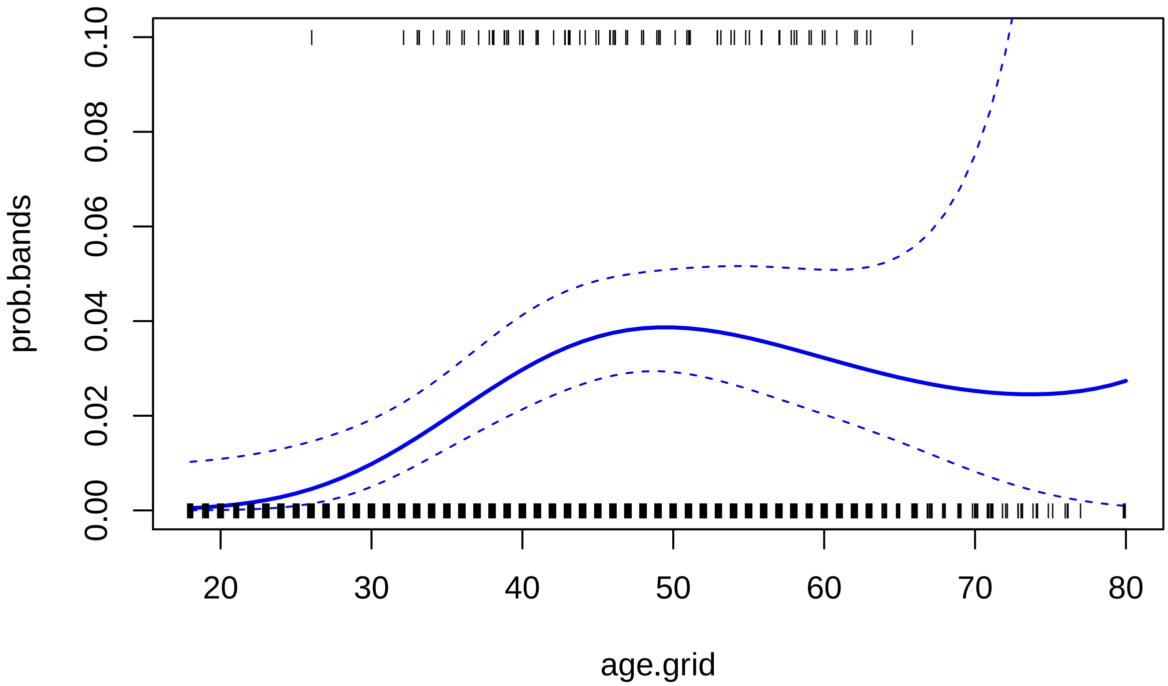
```
##         fit      lower     upper
## 1 -7.664756 -10.759826 -4.569686
## 2 -7.324776 -10.106699 -4.542852
## 3 -7.001732  -9.492821 -4.510643
## 4 -6.695229  -8.917158 -4.473300
## 5 -6.404868  -8.378691 -4.431045
```

We have done the computations on the logit scale. To transform we need to apply the inverse logit mapping

$$p = \frac{e^\eta}{1 + e^\eta}.$$

We can do this simultaneously for all three columns of `se.bands`:

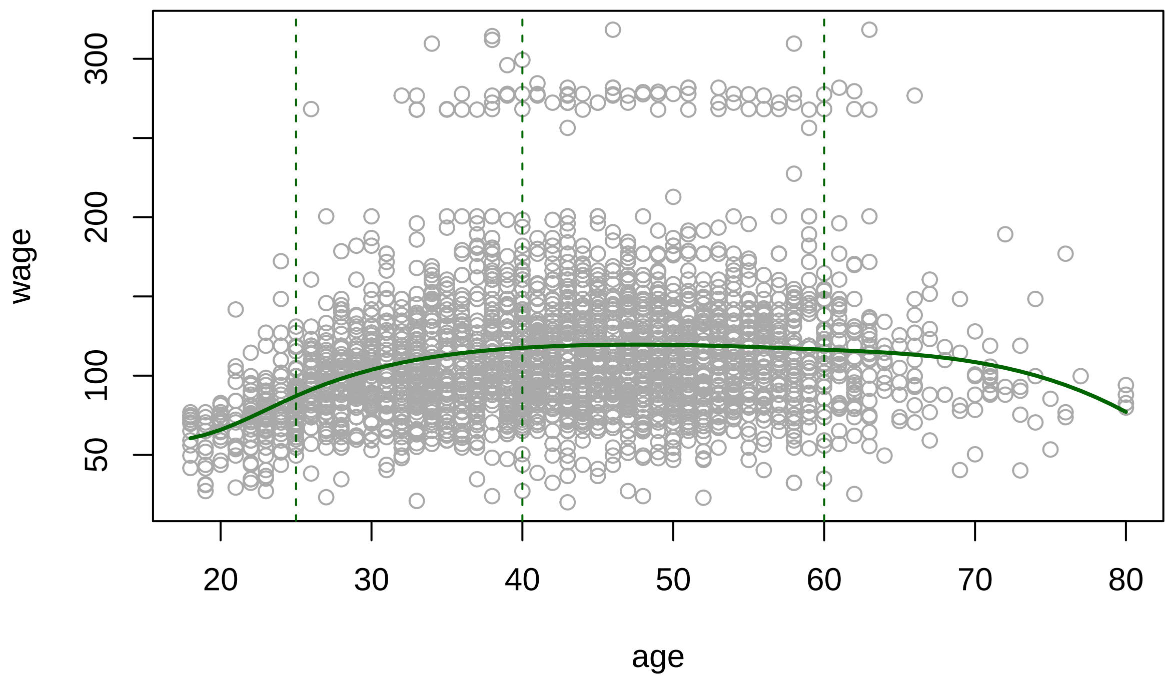
```
prob.bands <- exp(se.bands)/(1 + exp(se.bands))
matplot(age.grid, prob.bands, col="blue", lwd=c(2,1,1), lty=c(1,2,2), type="l", ylim=c(0,0.1))
points(jitter(age), I(wage>250)/10, pch="|", cex=0.5)
```



Splines

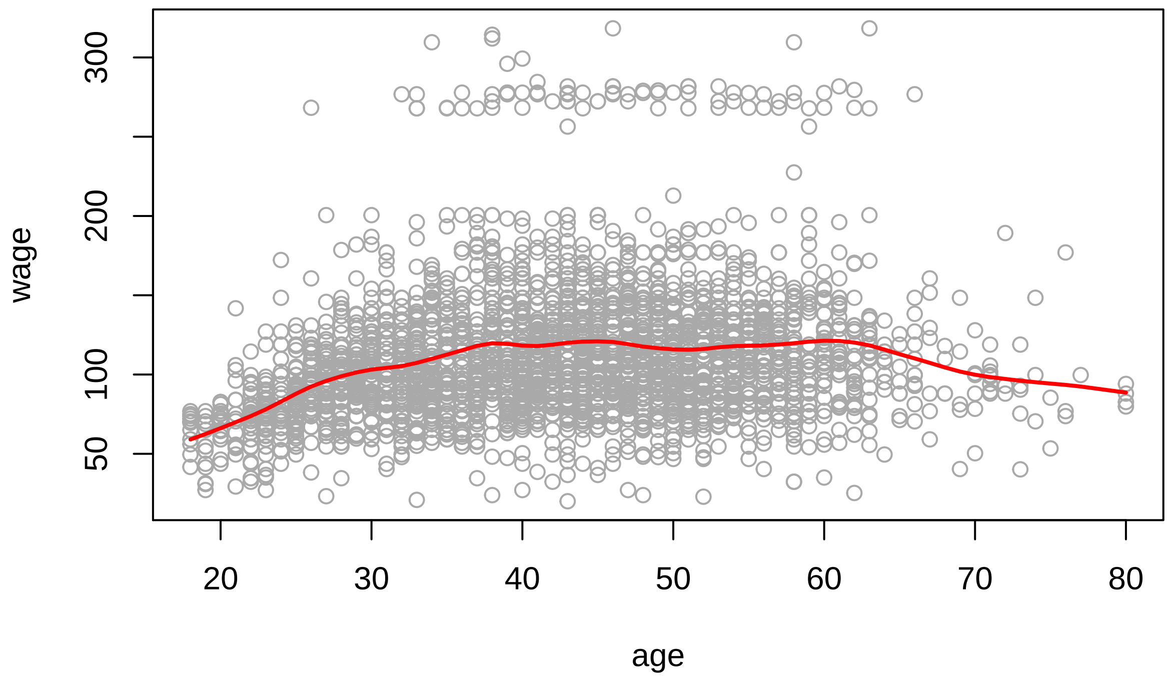
Splines are more flexible than polynomials, but the idea is rather similar. Here we will explore cubic splines.

```
library(splines)
fit <- lm(wage ~ bs(age, knots = c(25, 40, 60)), data = Wage)
plot(age, wage, col = "darkgrey")
lines(age.grid, predict(fit, list(age = age.grid)), col = "darkgreen", lwd = 2)
abline(v = c(25, 40, 60), lty = 2, col = "darkgreen")
```



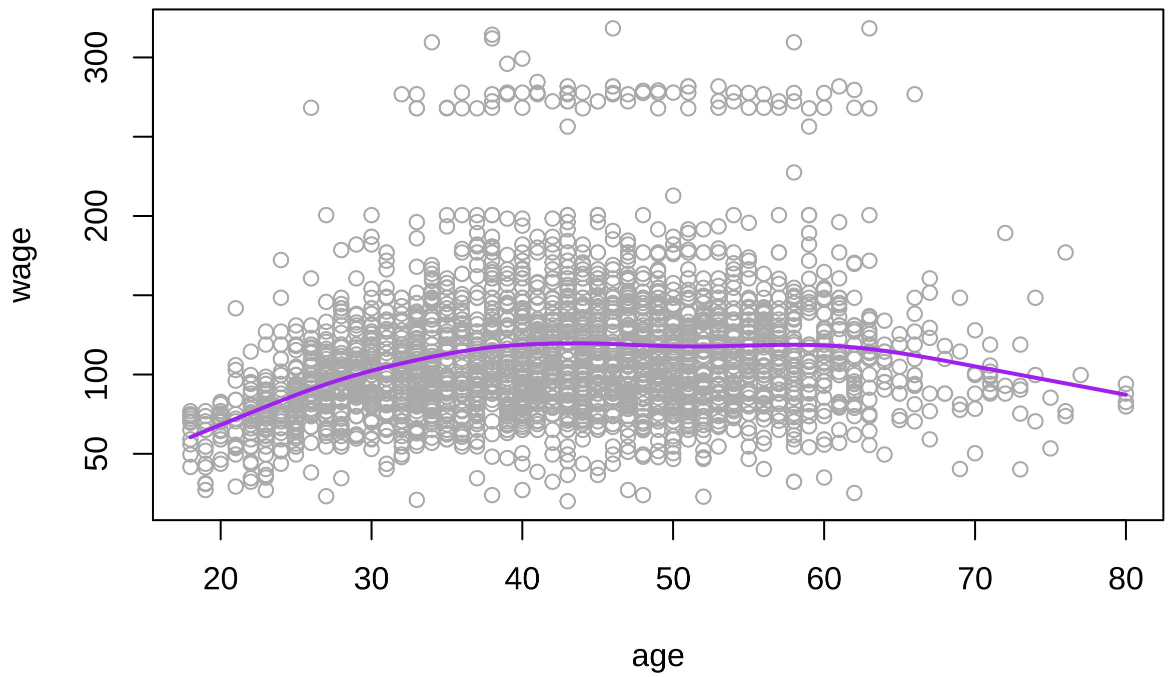
The smoothing splines does not require knot selection, but it does have a smoothing parameter, which can conveniently be specified via the effective degrees of freedom or `df`.

```
fit <- smooth.spline(age, wage, df = 16)
plot(age, wage, col = "darkgrey")
lines(fit, col = "red", lwd = 2)
```



Or we can use LOO cross-validation to select the smoothing parameter for us automatically:

```
fit <- smooth.spline(age, wage, cv = TRUE)
plot(age, wage, col = "darkgrey")
lines(fit, col = "purple", lwd = 2)
```




```
fit
```

```
## Call:
## smooth.spline(x = age, y = wage, cv = TRUE)
##
## Smoothing Parameter  spar= 0.6988943  lambda= 0.02792303 (12 iterations)
## Equivalent Degrees of Freedom (Df): 6.794596
## Penalized Criterion (RSS): 75215.9
## PRESS(l.o.o. CV): 1593.383
```

Generalized Additive Models

So far we have focused on fitting models with mostly single nonlinear terms. The `gam` package makes it easier to work with multiple nonlinear terms. In addition it knows how to plot these functions and their standard errors.

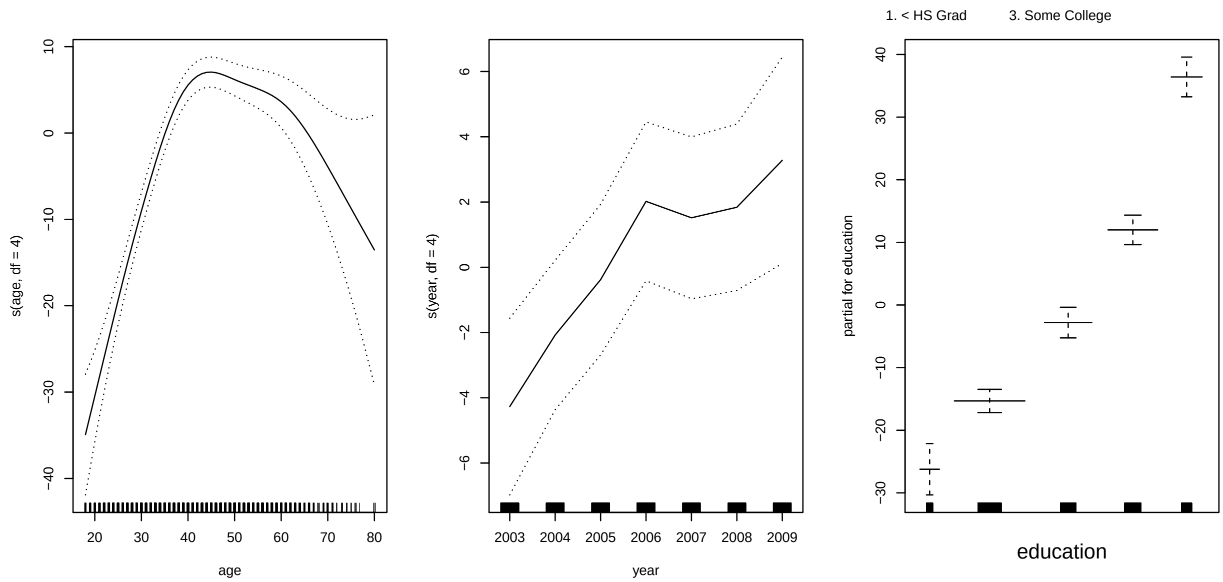
```
require(gam)
```

```
## Loading required package: gam
```

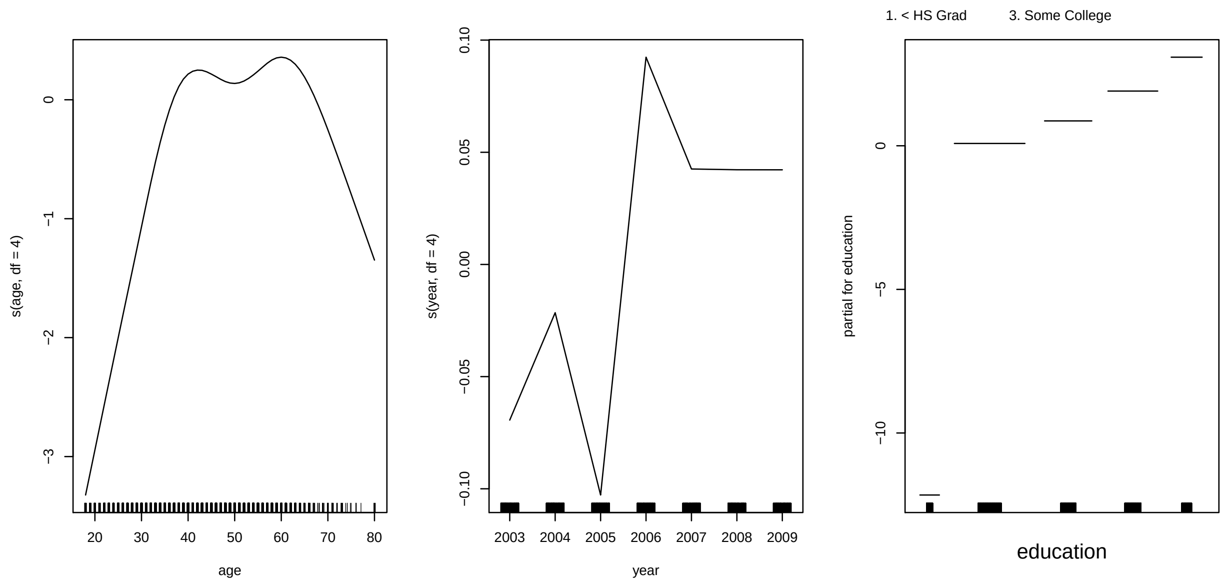
```
## Loading required package: foreach
```

```
## Loaded gam 1.14-4
```

```
gam1 <- gam(wage ~ s(age, df = 4) + s(year, df = 4) + education, data = Wage)
par(mfrow = c(1, 3))
plot(gam1, se = T)
```




```
gam2 <- gam(I(wage > 250) ~ s(age, df = 4) + s(year, df = 4) + education, data = Wage,
    family = binomial)
plot(gam2)
```



Lets see if we need a nonlinear terms for year

```
gam2a <- gam(I(wage > 250) ~ s(age, df = 4) + year + education, data = Wage,
    family = binomial)
anova(gam2a, gam2, test = "Chisq")
```

```
## Analysis of Deviance Table
##
## Model 1: I(wage > 250) ~ s(age, df = 4) + year + education
## Model 2: I(wage > 250) ~ s(age, df = 4) + s(year, df = 4) + education
```

```
##   Resid. Df Resid. Dev Df Deviance Pr(>Chi)
## 1      2990     603.78
## 2      2987     602.87  3  0.90498   0.8242
```

One nice feature of the `gam` package is that it knows how to plot the functions nicely, even for models fit by `lm` and `glm`.

```r
par(mfrow = c(1,3))
lm1 <- lm(wage ~ ns(age, df=4) + ns(year, df=4) + education, data = Wage)
plot.gam(lm1, se =T)
```