Nonlinear models: Polynomials and Splines

Explore nonlinear models using R tools.

```
require(ISLR)
```

```
## Loading required package: ISLR
```

```
attach(Wage)
```

Polynomials

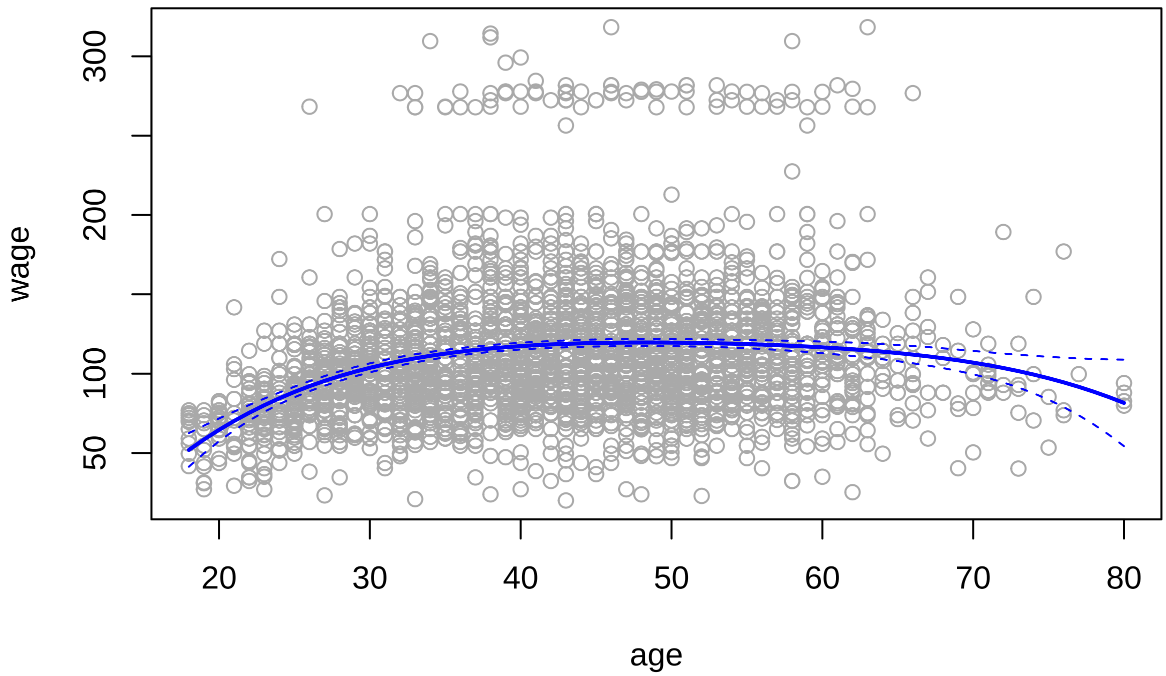
Focus on a single predictor, age:

```
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*. Let's 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])
pred = predict(fit, newdata = list(age=age.grid), se=T)
se.bands = cbind(pred$fit+2*pred$se,pred$fit-2*pred$se)
plot(age, wage, col="darkgrey")
lines(age.grid, pred$fit, lwd=2, col="blue")
matlines(age.grid, se.bands, col="blue", lty=2)
```



There are other ways of fitting a polynomials in R. For example:

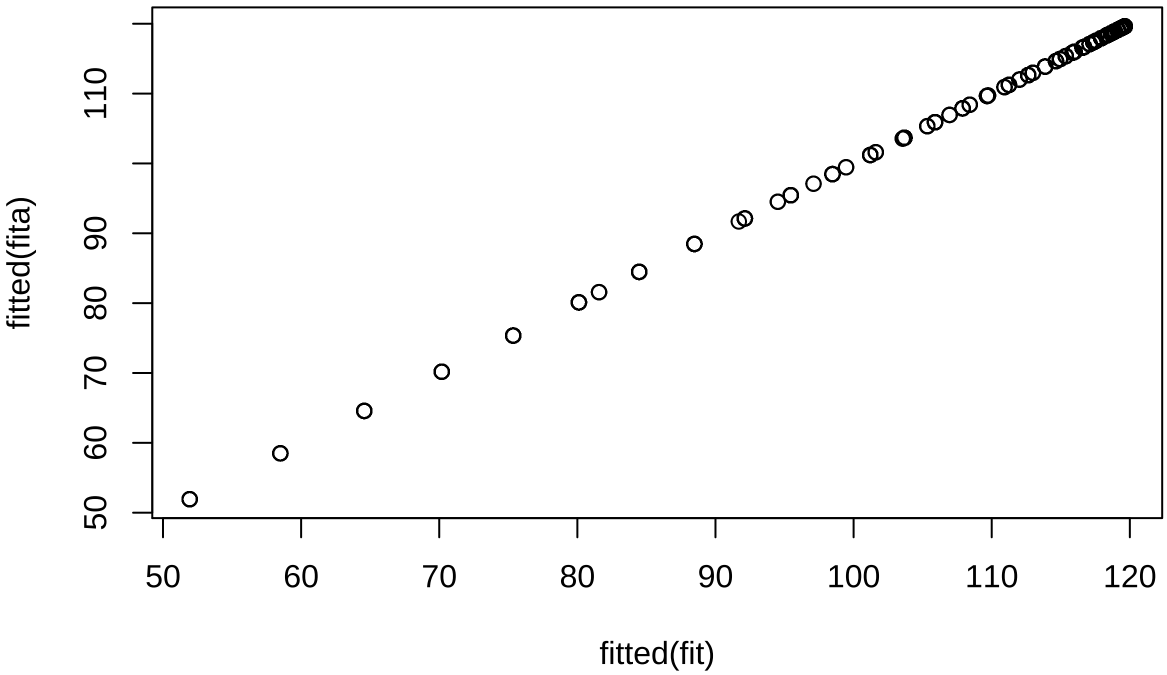
```r
fita = lm(wage~age+I(age^2)+I(age^3)+I(age^4), data=Wage)
summary(fita)
```

```
##
## 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
```

Above `I()` wrapper is used because `age^2` means something to the formula language, while `I(age^2)` is protected.

The coefficients are different, but the fits are the same.

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



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

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

```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

```
fita = glm(I(wage > 250) ~ poly(age,2), data=Wage, family=binomial)
fitb = glm(I(wage > 250) ~ poly(age,3), data=Wage, family=binomial)
anova(fita, fitb)
```

```
## Analysis of Deviance Table
##
## Model 1: I(wage > 250) ~ poly(age, 2)
## Model 2: I(wage > 250) ~ poly(age, 3)
##   Resid. Df Resid. Dev Df Deviance
## 1      2997     709.02
## 2      2996     707.92  1   1.1022
```

```
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
```

```
preds = predict(fitb, 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,]
```

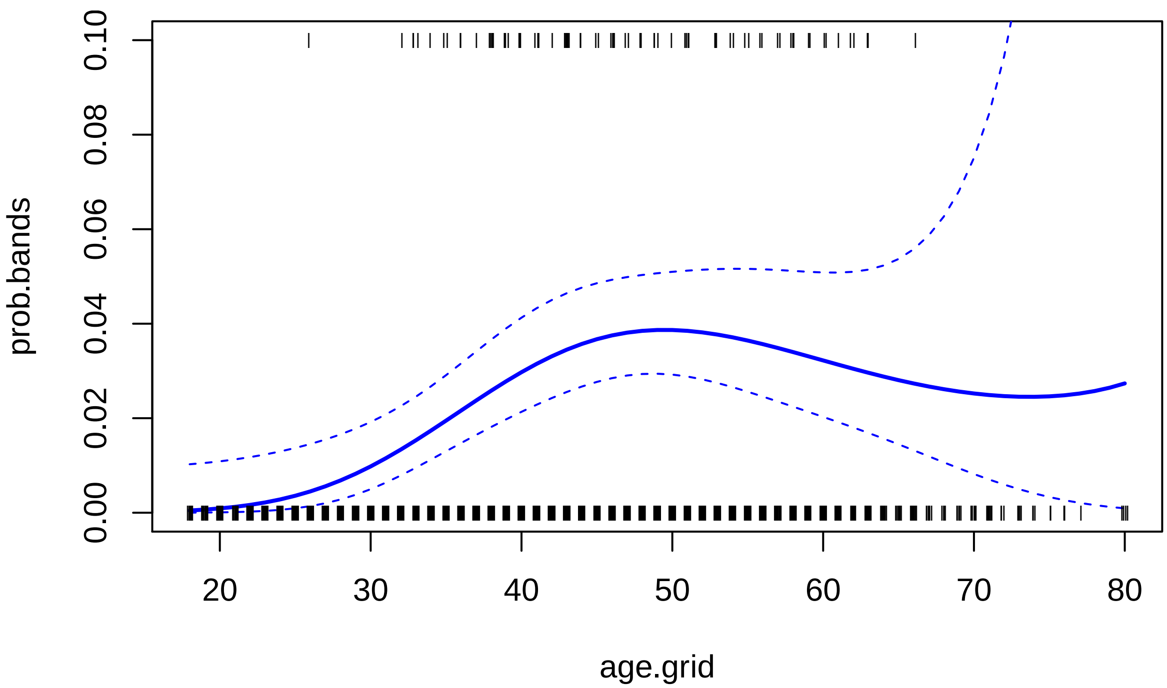
```
##         fit      lower     upper
## 1 -7.664756 -10.759826 -4.569686
## 2 -7.324776 -10.106699 -4.542852
## 3 -7.001732  -9.492821 -4.510643
## 4 -6.695229  -8.917158 -4.473300
## 5 -6.404868  -8.378691 -4.431045
```

The above calculations are on the logit scale. We need to transform it back using the inverse logit

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

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.

```
require(splines)
```

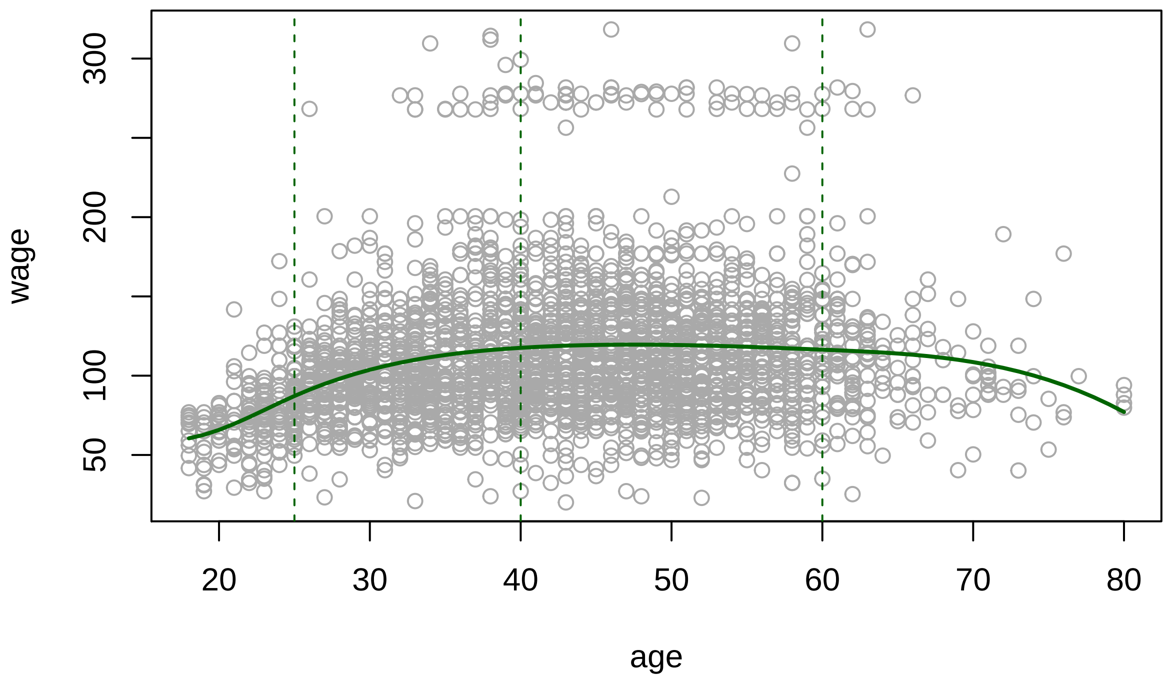
```
## Loading required package: splines
```

```
fit = lm(wage~bs(age, knots=c(25,40,60)), data=Wage)
summary(fit)
```

```
##
## Call:
## lm(formula = wage ~ bs(age, knots = c(25, 40, 60)), data = Wage)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -98.832 -24.537  -5.049  15.209 203.207
##
```

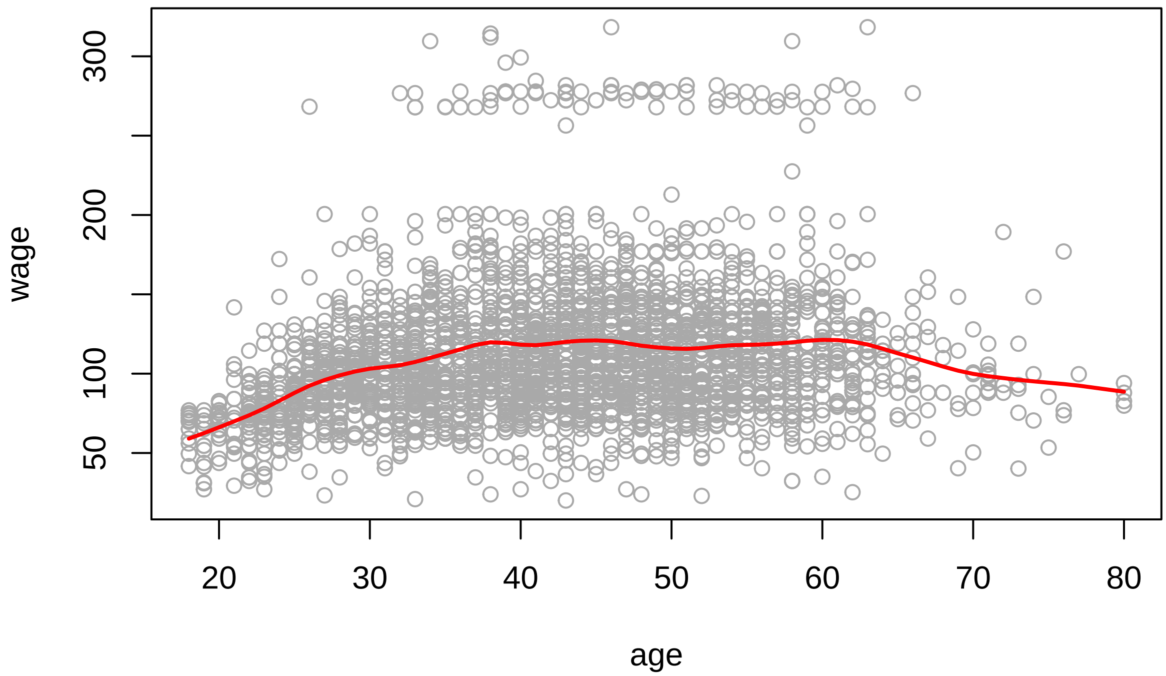
```
## Coefficients:
##                               Estimate Std. Error t value Pr(>|t|)
## (Intercept)                     60.494      9.460   6.394 1.86e-10 ***
## bs(age, knots = c(25, 40, 60))1    3.980     12.538   0.317 0.750899
## bs(age, knots = c(25, 40, 60))2   44.631      9.626   4.636 3.70e-06 ***
## bs(age, knots = c(25, 40, 60))3   62.839     10.755   5.843 5.69e-09 ***
## bs(age, knots = c(25, 40, 60))4   55.991     10.706   5.230 1.81e-07 ***
## bs(age, knots = c(25, 40, 60))5   50.688     14.402   3.520 0.000439 ***
## bs(age, knots = c(25, 40, 60))6   16.606     19.126   0.868 0.385338
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 39.92 on 2993 degrees of freedom
## Multiple R-squared:  0.08642,    Adjusted R-squared:  0.08459
## F-statistic: 47.19 on 6 and 2993 DF,  p-value: < 2.2e-16
```

```r
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 don't require knot selection, but they do have a smoothing parameter, which can be conveniently specified via the effective degrees of freedom or `df`.

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

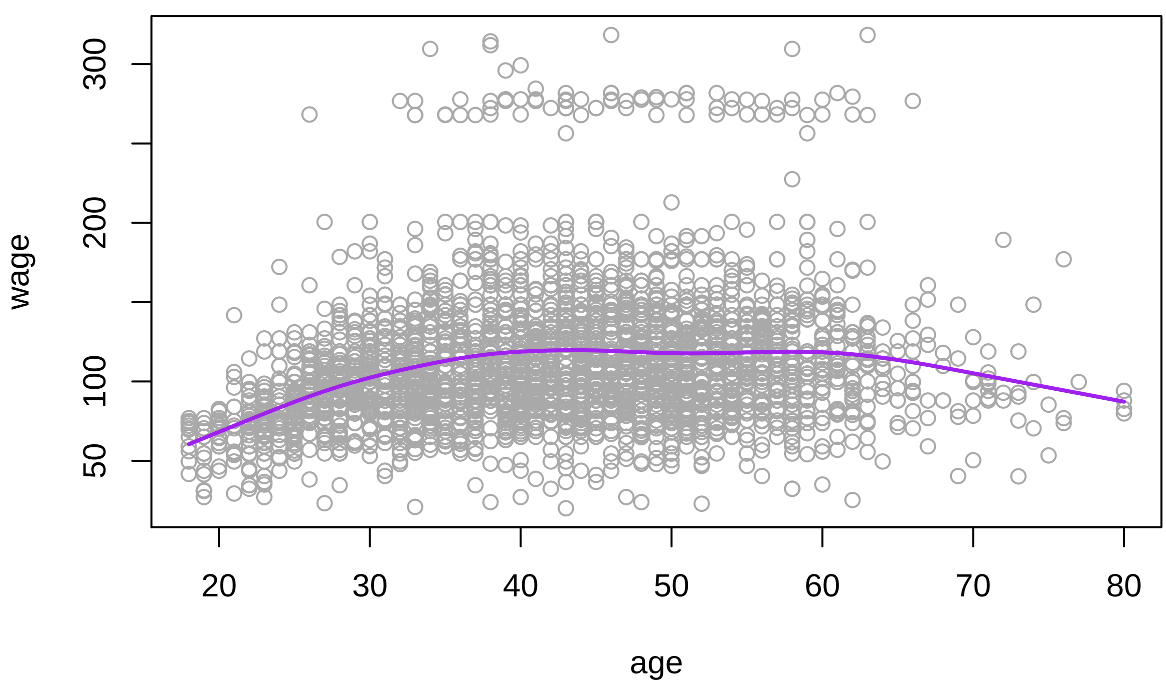


Or we can use LOO cross-validation to select the smoothing parameter for us automatically:

```
fit = smooth.spline(age, wage, cv=T)
```

```
## Warning in smooth.spline(age, wage, cv = T): cross-validation with non-
## unique 'x' values seems doubtful
```

```
plot(age, wage, col="darkgrey")
lines(fit, col="purple", lwd=2)
```



```r
fit
```

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

Generalized Additive Models

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

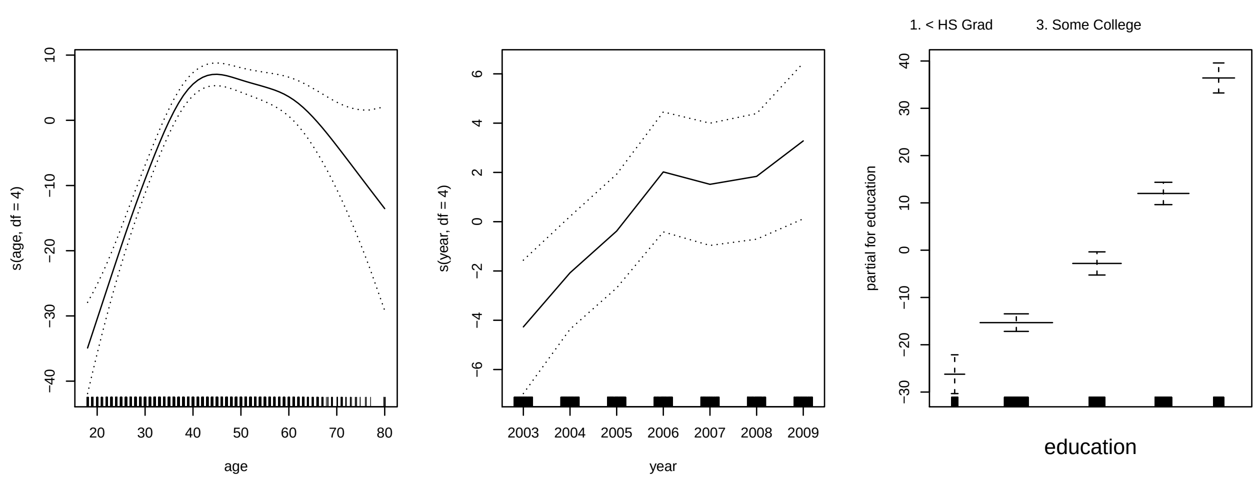
```r
require(gam)
```

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

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

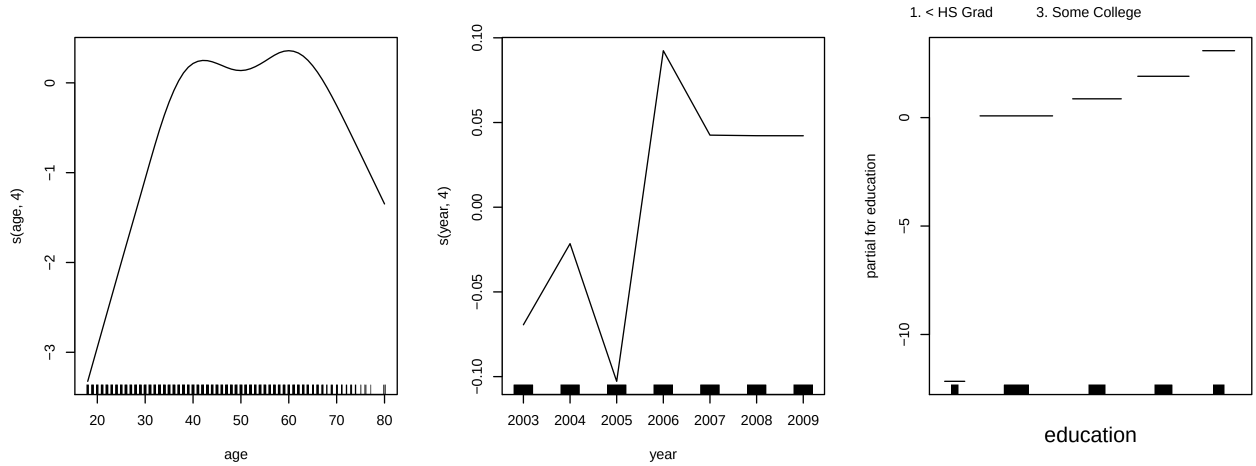
```
## Loaded gam 1.12
```

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



Let's do the same, but now with logistic regression:

```r
require(gam)
gam2 = gam(I(wage>250)~s(age,4)+s(year,4)+education, data=Wage, family = binomial)
par(mfrow=c(1,3))
plot(gam2)
```



Let's see if we need a nonlinear terms for year

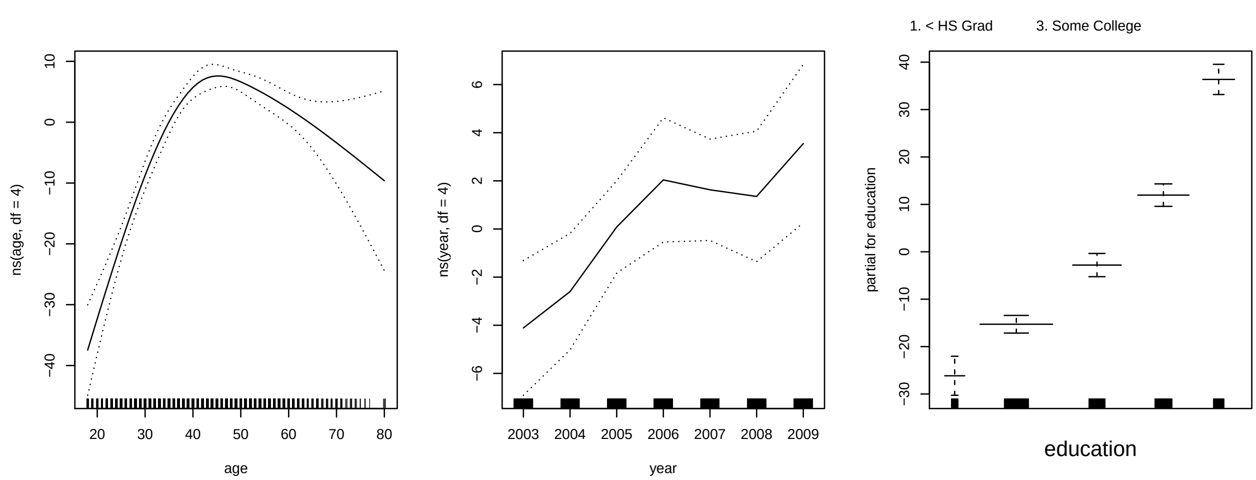
```
gam2a = gam(I(wage>250)~s(age,4)+year+education, data=Wage, family=binomial)
anova(gam2a,gam2,test="Chisq")
```

```
## Analysis of Deviance Table
##
## Model 1: I(wage > 250) ~ s(age, 4) + year + education
## Model 2: I(wage > 250) ~ s(age, 4) + s(year, 4) + education
##   Resid. Df Resid. Dev Df Deviance Pr(>Chi)
## 1      2990     603.78
## 2      2987     602.87  3  0.90498   0.8242
```

The p-value is very high the nonlinear `year` term, so we don't need it. We may not even need `year`.

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

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



See the chapter on `gam` for more in Introduction to Statistical Learning.