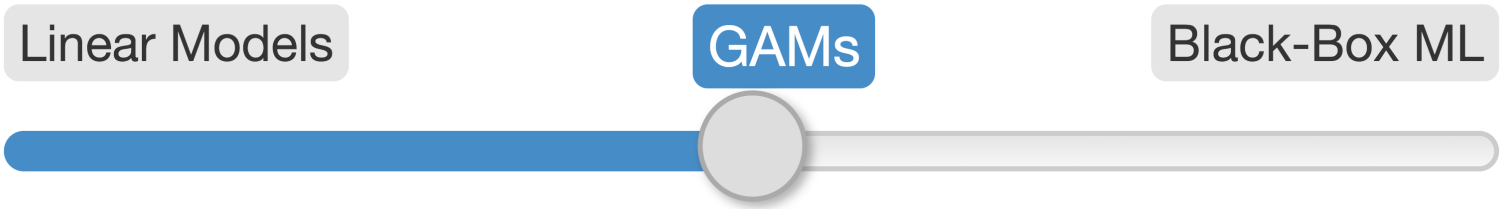
Nonlinear Modeling II

Generalized Additive Models (close to chapter 7, ISLR)

M Loecher

Contents

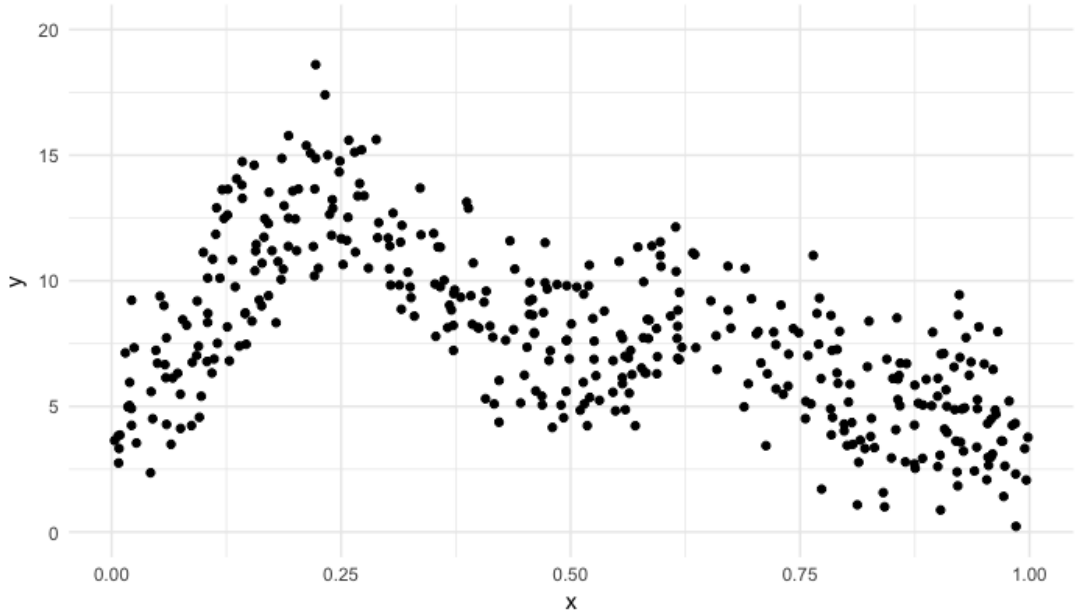
Trade-offs in Model Building



Pros and Cons of GAMs

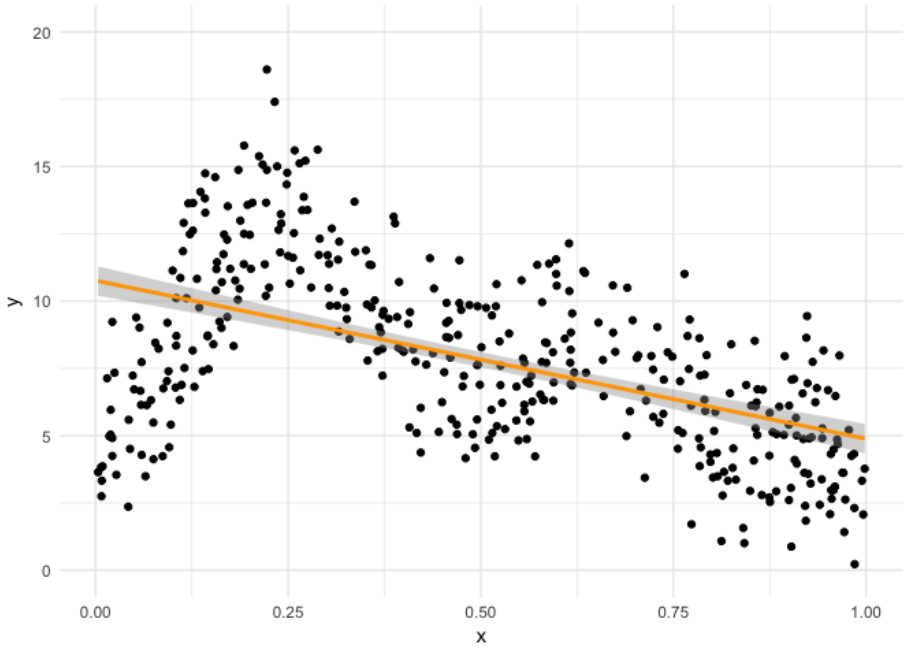
+ GAMs allow us to fit a non-linear f_j to each X_j, so that we can automatically model non-linear relationships that standard linear regression will miss. This means that we do not need to manually try out many different transformations on each variable individually.
+ The non-linear fits can potentially make more accurate predictions for the response Y .
+ Because the model is additive, we can still examine the effect of each X_j on Y individually while holding all of the other variables fixed. Hence if we are interested in inference, GAMs provide a useful representation.
+ The smoothness of the function f_j for the variable X_j can be summarized via degrees of freedom.
- The main limitation of GAMs is that the model is restricted to be additive. With many variables, important interactions can be missed. However, as with linear regression, we can manually add interaction terms to the GAM model by including additional predictors of the form X_jÖX_k. In addition we can add low-dimensional interaction functions of the form $f_{jk}(X_j, X_k)$ into the model; such terms can be fit using two-dimensional smoothers such as local regression, or two-dimensional splines (not covered here).

Non-linear Relationships



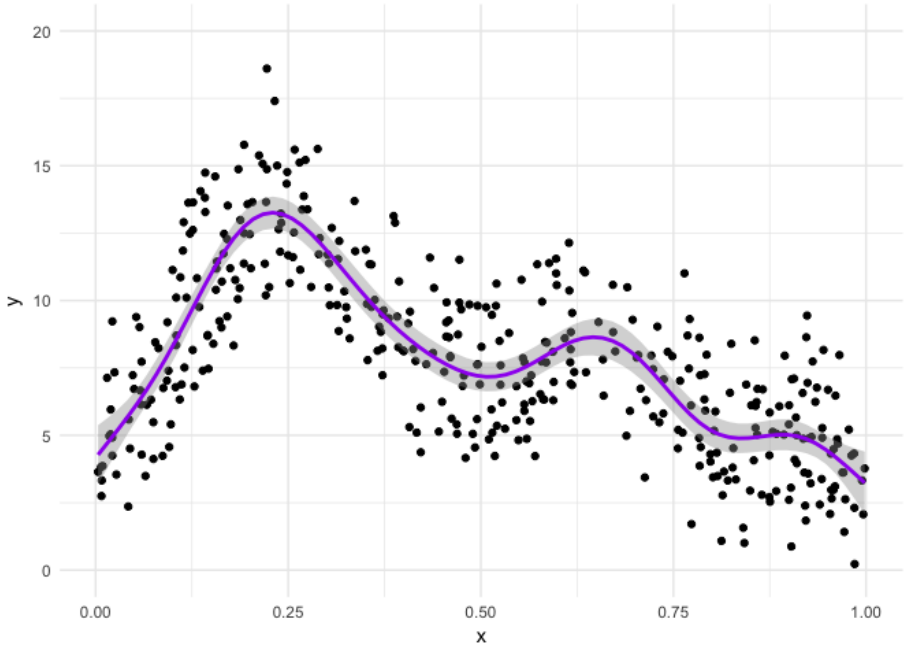
Nonlinear Relationships (2)

```
linear_mod <- lm(y ~ x, data = my_data)
```

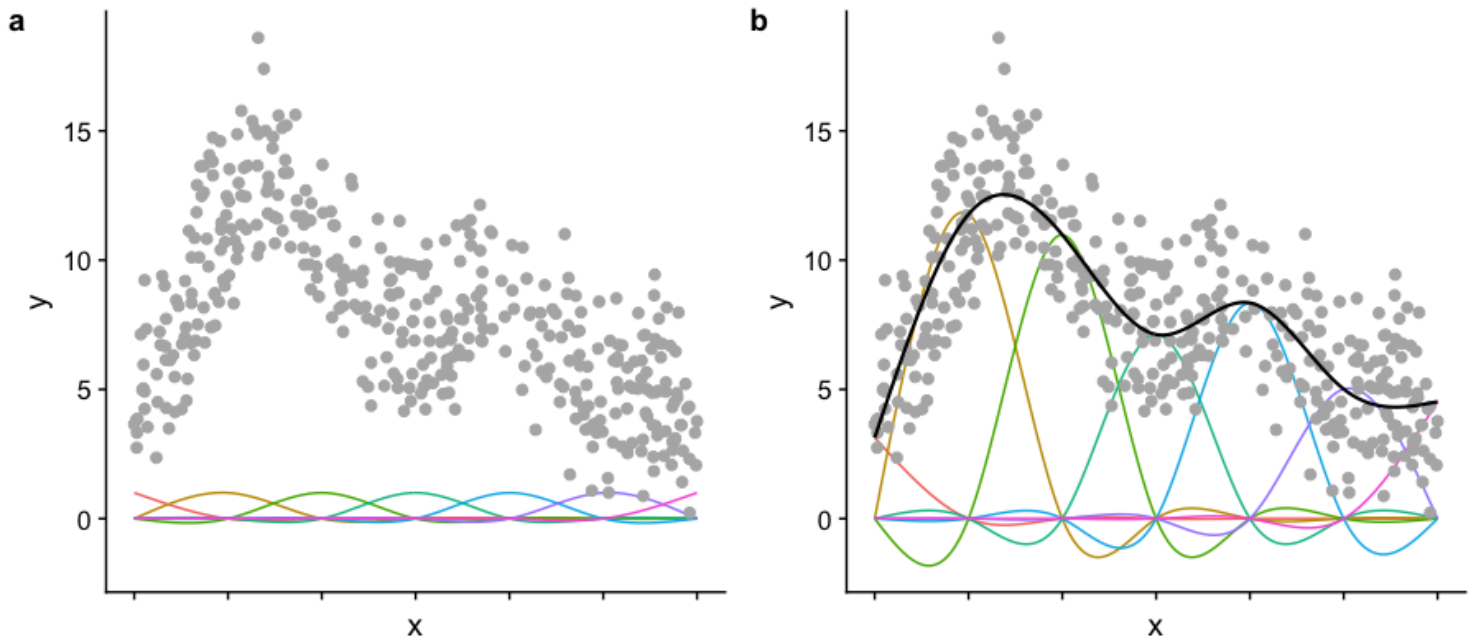


Nonlinear Relationships (3)

```
library(mgcv)
gam_mod <- gam(y ~ s(x), data = my_data)
```



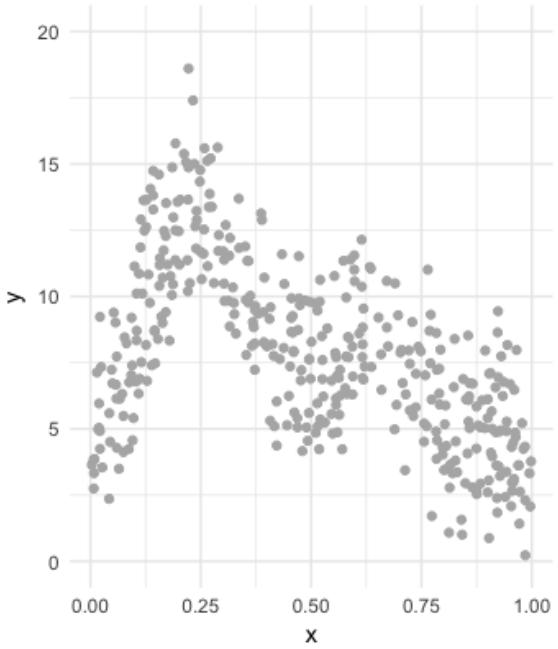
Basis Functions



Basis Functions (2)

```
gam_mod <- gam(y ~ s(x), data = my_data)

coef(gam_mod)

(Intercept)      s(x2).1      s(x2).2
7.814448         5.272290     5.104941

s(x2).3          s(x2).4      s(x2).5
1.271135         1.720561    -1.180613

s(x2).6
-2.676133
```

Getting the right fit

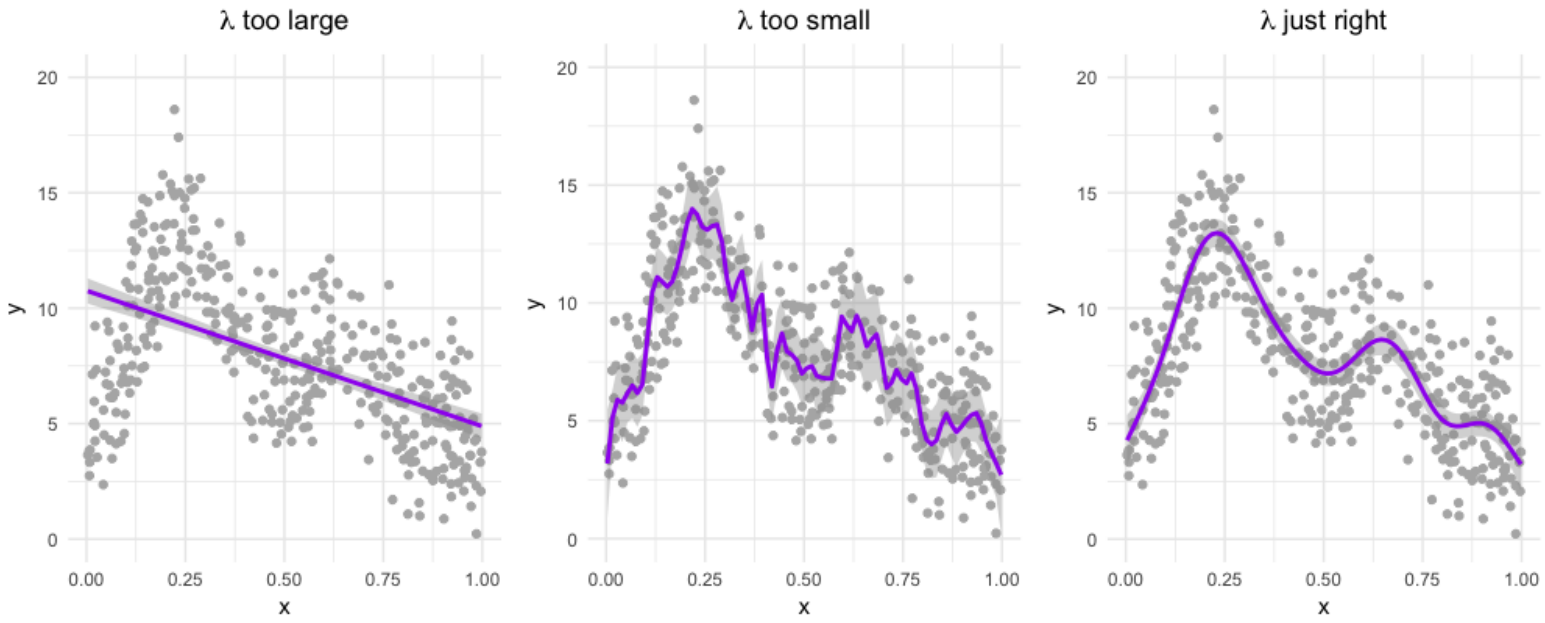


- Close to the data (avoiding under-fitting)
- Not fitting the noise (avoiding over-fitting)

Balancing Wiggliness

$$\text{Fit} = \text{Likelihood} - \lambda \times \text{Wiggliness}$$

Choosing the Right Smoothing Parameter



Smoothing Syntax

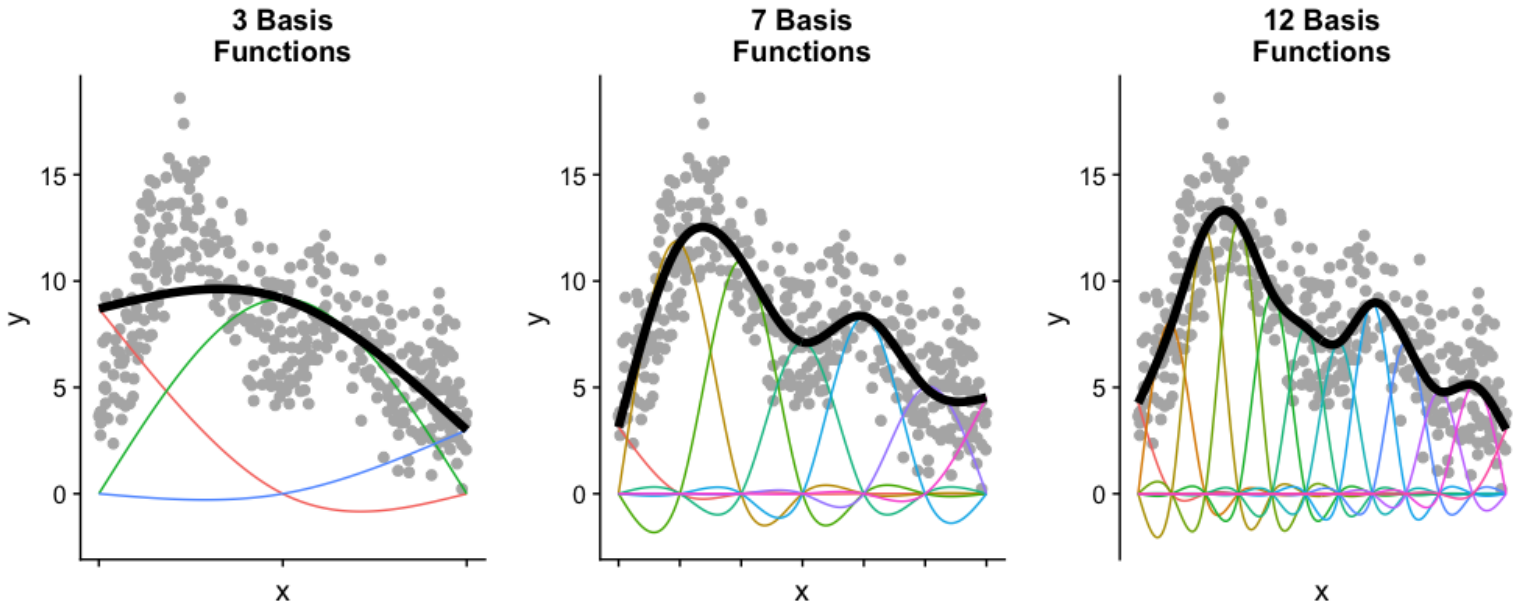
Setting a fixed smoothing parameter

```
gam(y ~ s(x), data = dat, sp = 0.1)
gam(y ~ s(x, sp = 0.1), data = dat)
```

Smoothing via restricted maximum likelihood

```
gam(y ~ s(x), data = dat, method = "REML")
```

Number of basis functions



Basis Function Syntax

Setting number of basis functions

```
gam(y ~ s(x, k = 3), data = dat, method = "REML")

gam(y ~ s(x, k = 10), data = dat, method = "REML")
```

Use the defaults

```
gam(y ~ s(x), data = dat, method = "REML")
```

GAM Exercises part I

Multiple Smooths

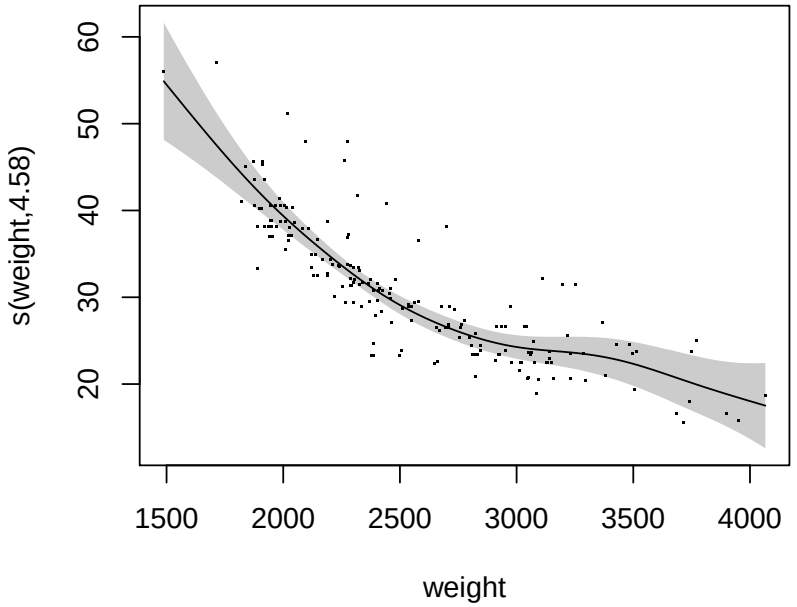
A true understanding of the label *additive* only comes in the context of multiple variables. A GAM is an extension of the multiple linear regression model which allows for non-linear relationships between each feature and the response. We simply replace each linear component $\beta_j x_{ij}$ with a (smooth) nonlinear function $f_j(x_{ij})$ so that the model becomes:

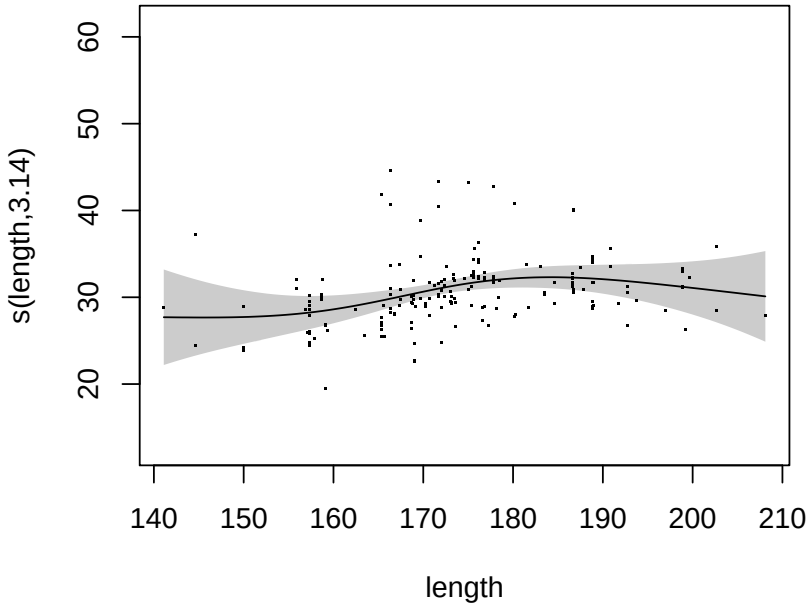
$$y_i = \beta_0 + f_1(x_{i1}) + f_2(x_{i2}) \ldots + f_p(x_{ip}) + \epsilon_i = \beta_0 + \sum_{j=1}^{p} f_j(x_{ij}) + \epsilon_i$$

Our Working Dataset: mpg

make	fuel	aspir	doors	style	drive	eng.loc	wb	length	width	height	weight	eng.type	cylinders	eng.cc	fuel.sys	bore	stroke
alfa-romero	gas	std	two	convertible	rwd	front	88.6	168.8	64.1	48.8	2548	dohc	four	130	mpfi	3.47	2.68
alfa-romero	gas	std	two	convertible	rwd	front	88.6	168.8	64.1	48.8	2548	dohc	four	130	mpfi	3.47	2.68
alfa-romero	gas	std	two	hatchback	rwd	front	94.5	171.2	65.5	52.4	2823	ohcv	six	152	mpfi	2.68	3.47
audi	gas	std	four	sedan	fwd	front	99.8	176.6	66.2	54.3	2337	ohc	four	109	mpfi	3.19	3.40
audi	gas	std	four	sedan	4wd	front	99.4	176.6	66.4	54.3	2824	ohc	five	136	mpfi	3.19	3.40
audi	gas	std	two	sedan	fwd	front	99.8	177.3	66.3	53.1	2507	ohc	five	136	mpfi	3.19	3.40

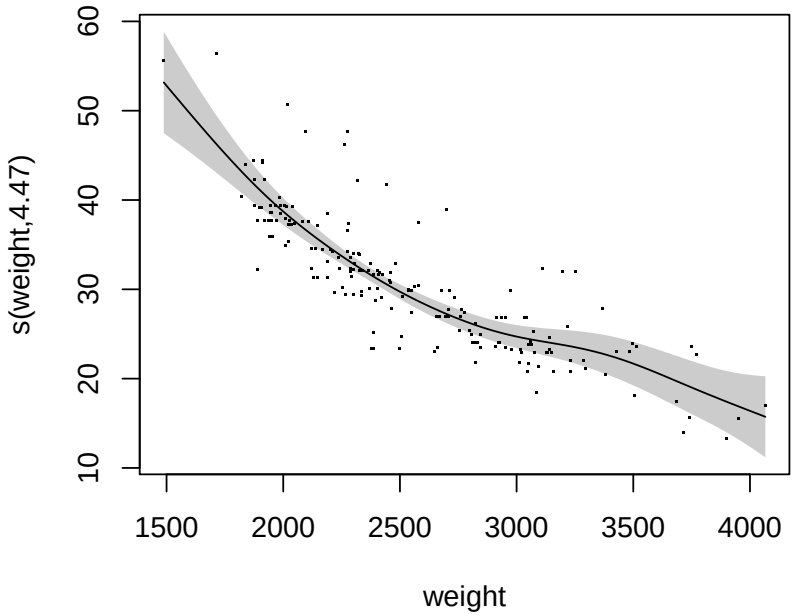
```
mod2 <- gam(hw.mpg ~ s(weight) + s(length) , data = mpg, method = "REML")
```

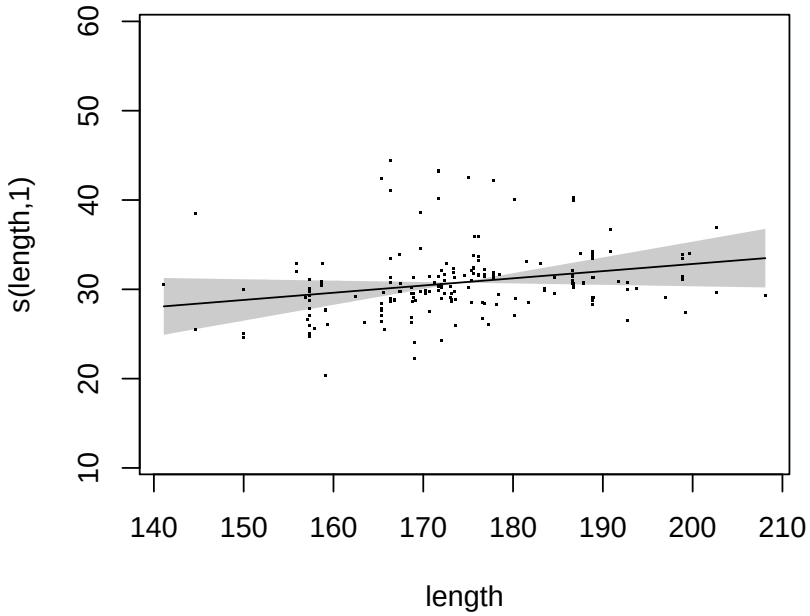




Linear Terms I

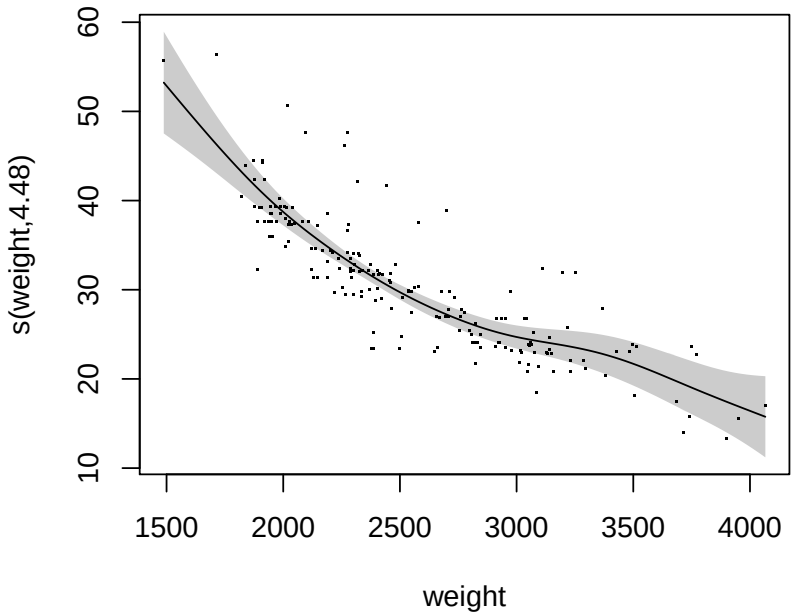
```
mod3 <- gam(hw.mpg ~ s(weight) + length , data = mpg, method = "REML")
```

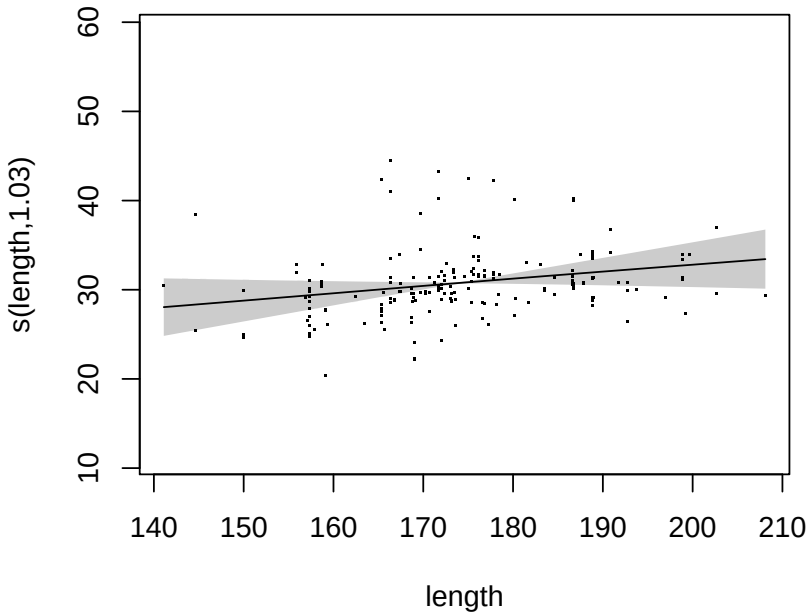




Linear Terms II

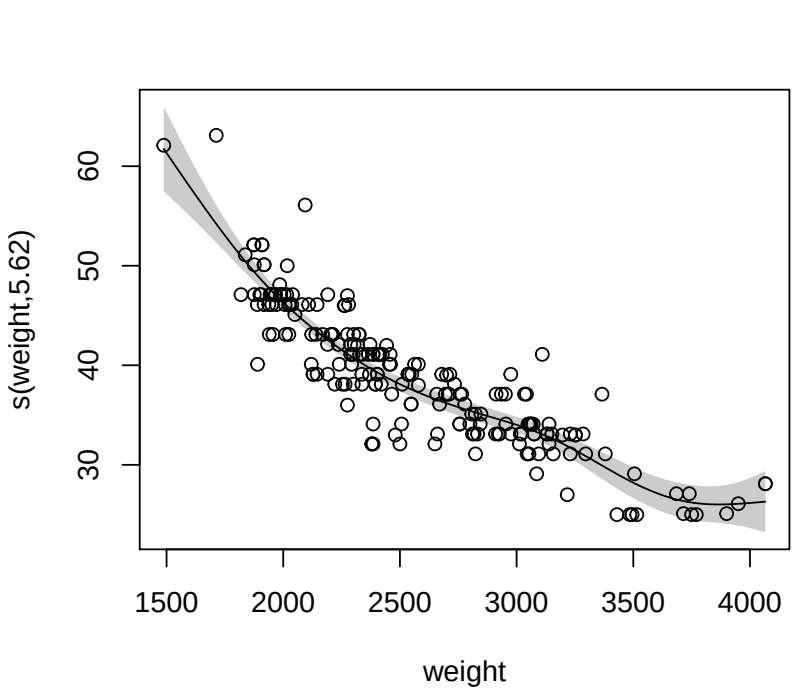
```
mod4 <- gam(hw.mpg ~ s(weight) + s(length,sp=100) , data = mpg, method = "REML")
```

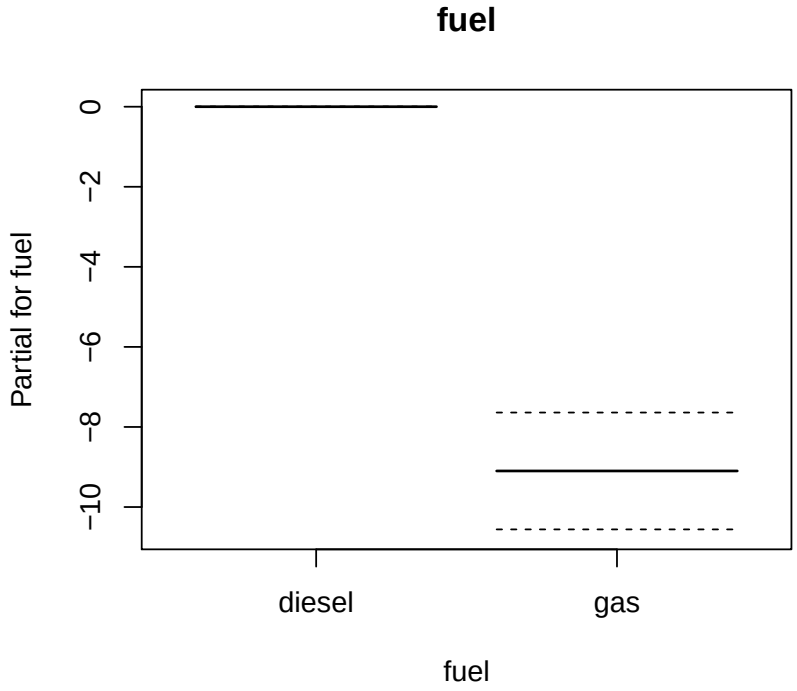




Categorical Terms I

```
mod5 <- gam(hw.mpg ~ s(weight) + fuel , data = mpg, method = "REML")
```



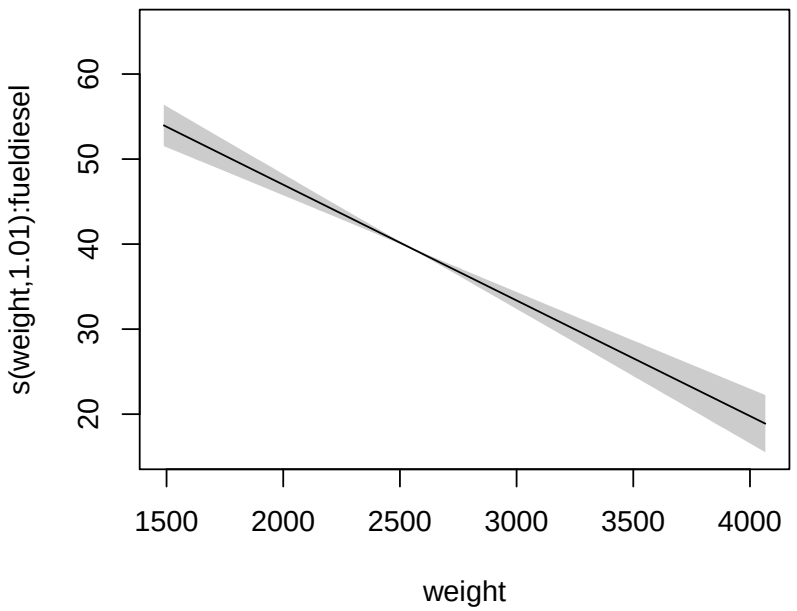


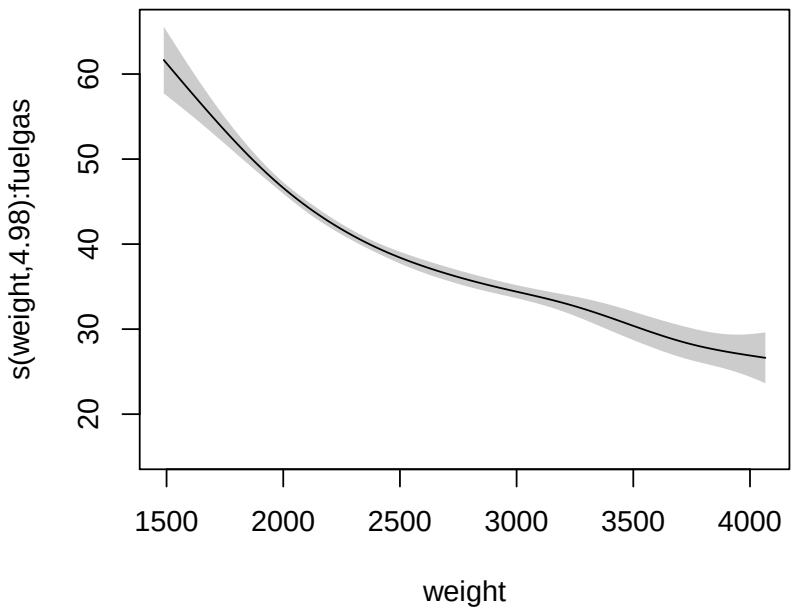
In this model the nonlinear effects of weight is the same for both fuel types. (You coulod view this as the analogy of the fixed slope, different intercepts in linear models!)

Categorical Terms II

We can also specify different smooths for different levels of teh categorical variable! ("a factor smooth interaction")

```
mod6 <- gam(hw.mpg ~ s(weight, by= fuel) + fuel, data = mpg, method = "REML")
```





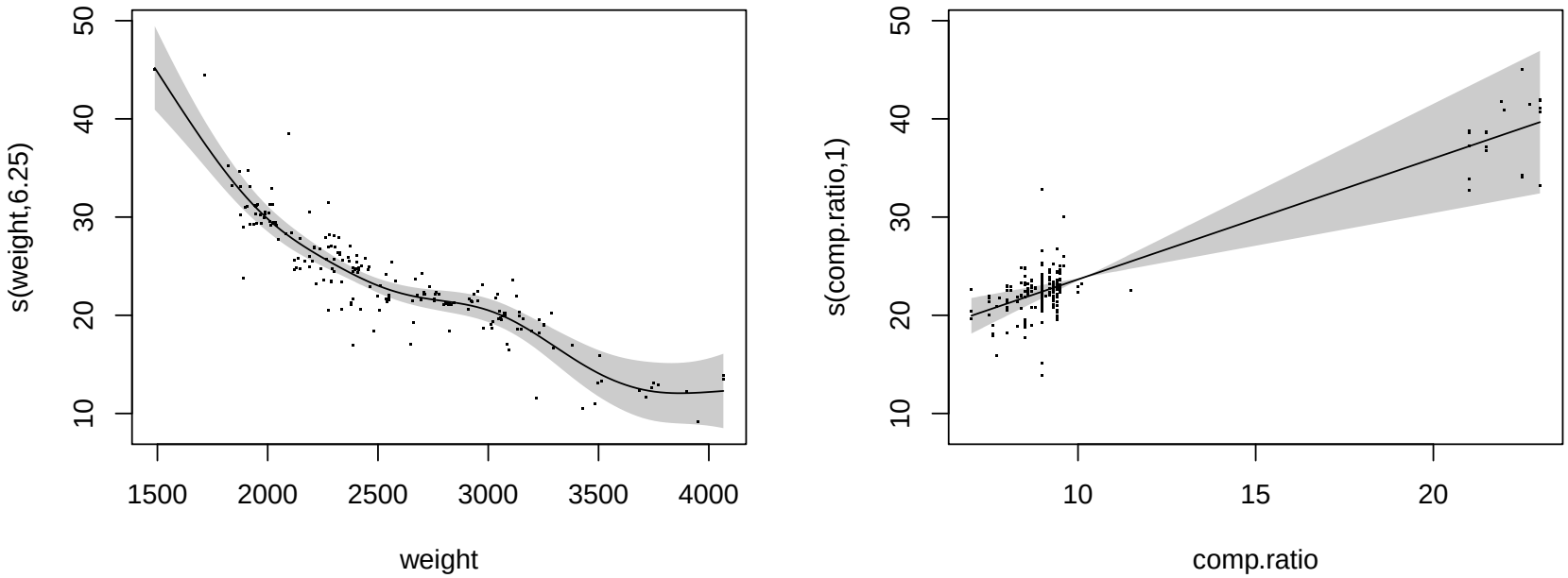
Interpreting GAM outputs

```
mod_city4 <- gam(hw.mpg ~ s(weight) +  s(price) + s(rpm) + s(comp.ratio) + s(widt
                 + fuel , data = mpg, method = "REML")
summary(mod_city4)
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## hw.mpg ~ s(weight) + s(price) + s(rpm) + s(comp.ratio) + s(width) +
##     fuel
##
## Parametric coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   23.873      3.531   6.760 1.89e-10 ***
## fuelgas        7.571      3.922   1.931   0.0551 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##
## Approximate significance of smooth terms:
##                   edf Ref.df      F  p-value
## s(weight)     6.254  7.439 20.909  < 2e-16 ***
## s(price)      2.681  3.421  1.678    0.155
## s(rpm)        7.499  8.285  8.534 2.07e-09 ***
## s(comp.ratio) 1.000  1.001 18.923 2.22e-05 ***
## s(width)      1.001  1.001  0.357    0.551
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =   0.89   Deviance explained = 90.1%
## -REML = 464.81  Scale est. = 5.171     n = 199
```

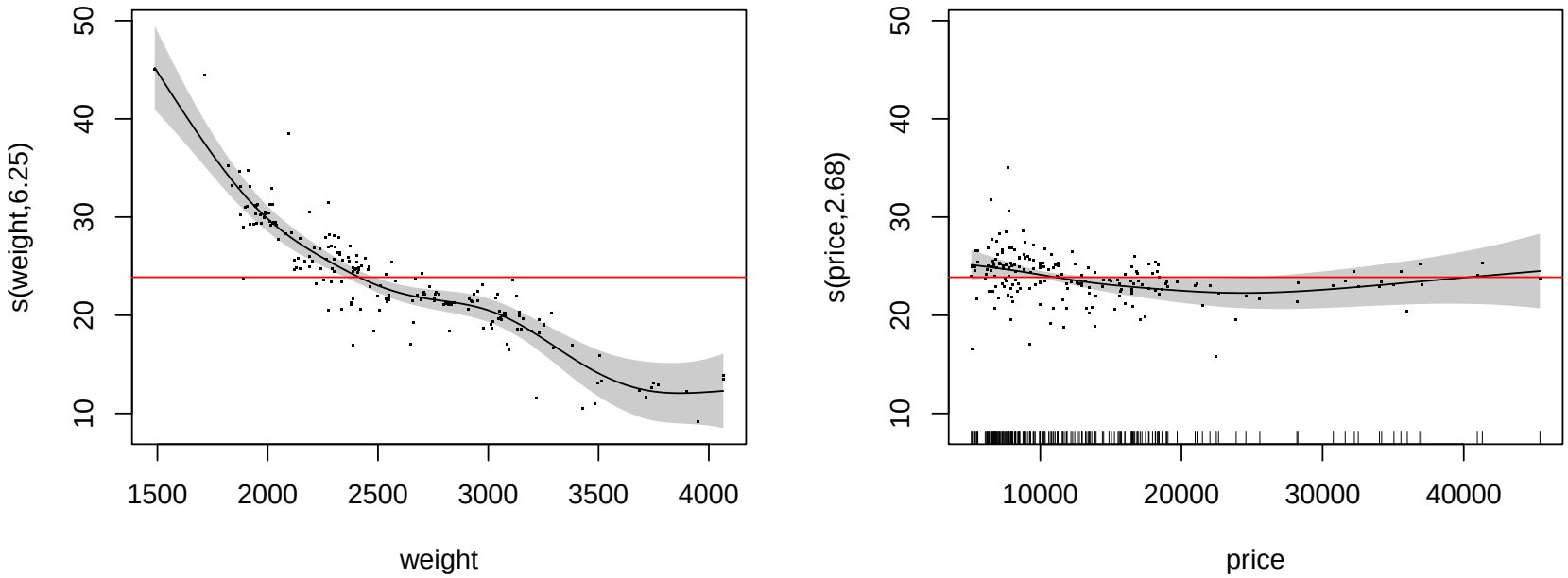
Effective Degrees of Freedom



Significance of Smooth Terms

Overall significance of smooth. p-values are approximate.

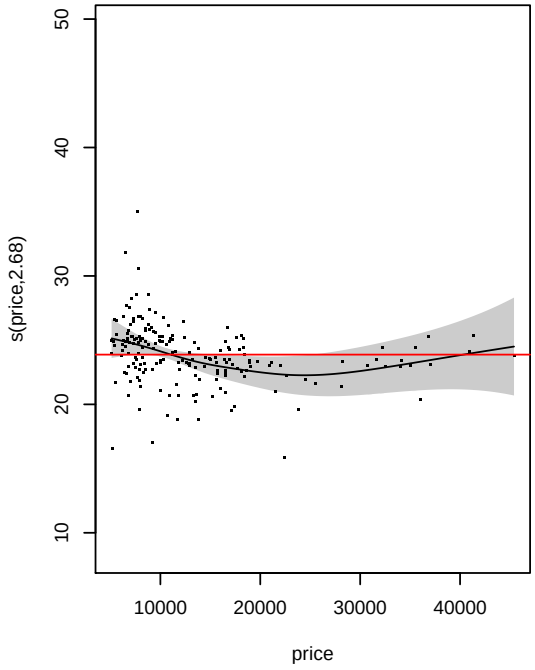
One way to interpret significance: you cannot draw a horizontal line through the 95% confidence interval.

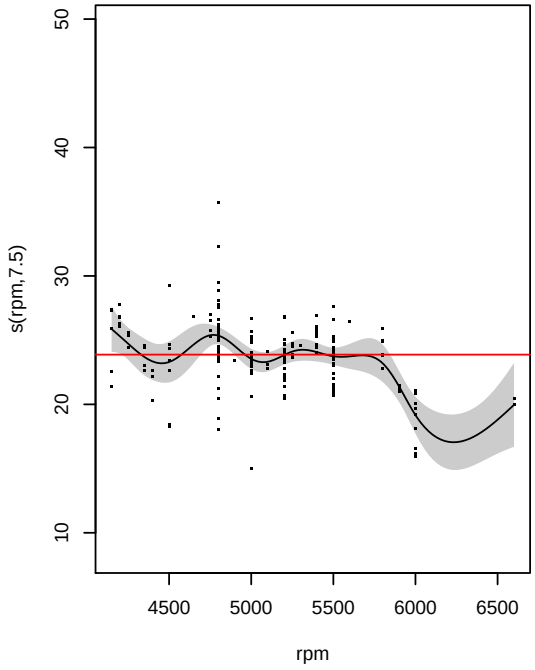


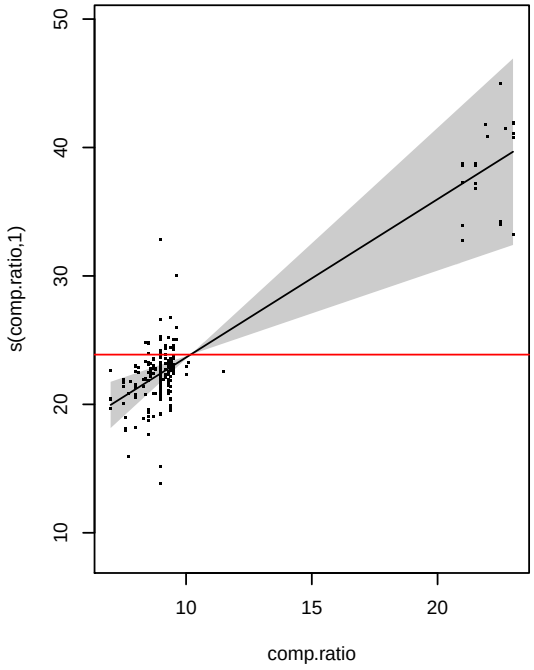
Significance and Effective Degress of Freedom

Two separate concepts, one does not imply the other !

	edf	Ref.df	F	p-value
s(weight)	6.254138	7.439475	20.909403	0.0000000
s(price)	2.681086	3.421421	1.678134	0.1549673
s(rpm)	7.499029	8.285177	8.533672	0.0000000
s(comp.ratio)	1.000337	1.000650	18.922944	0.0000222
s(width)	1.000696	1.001337	0.357271	0.5506887



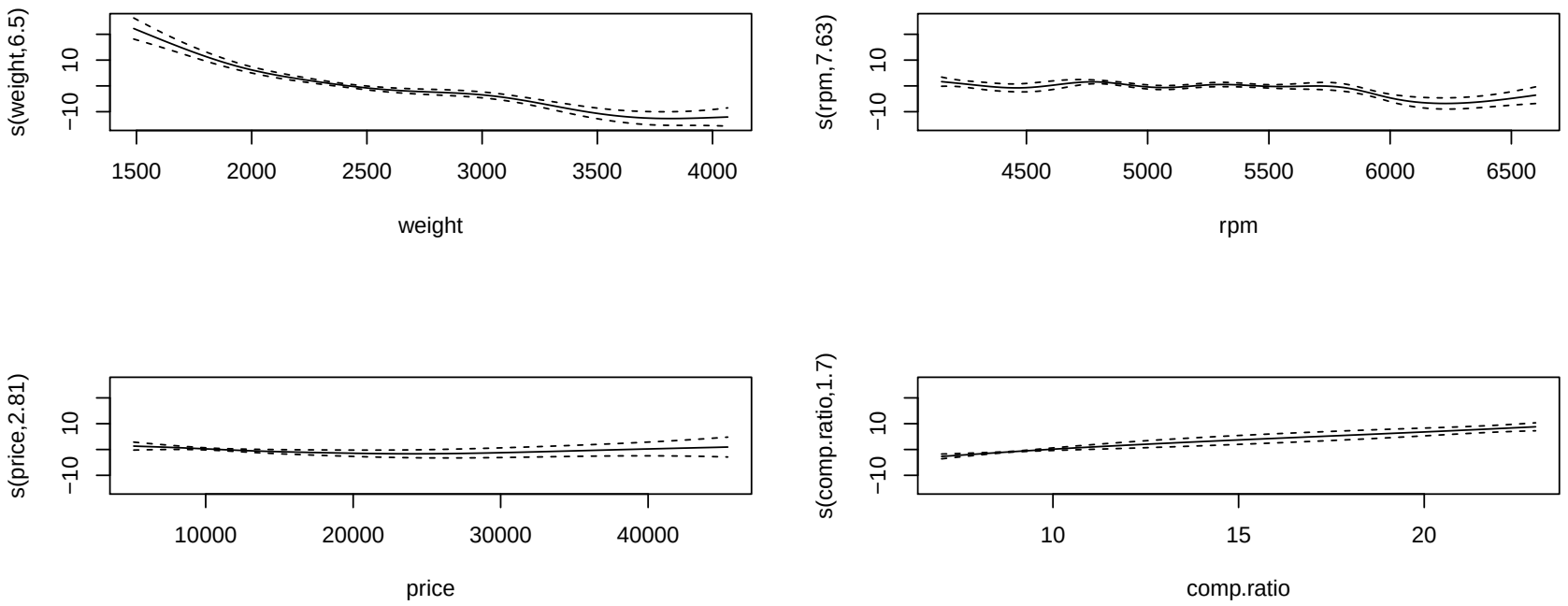




Visualizing GAMs

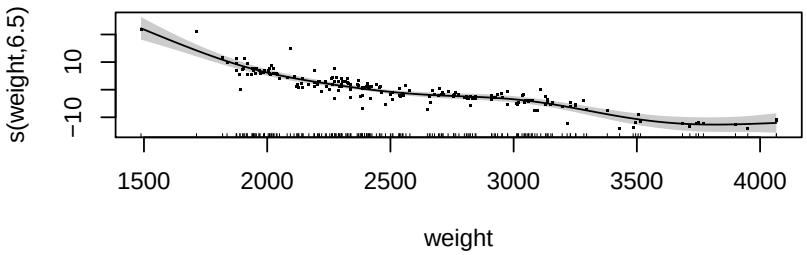
```
gam_mod <- gam(hw.mpg ~ s(weight) +  s(rpm) + s(price) + s(comp.ratio) , data = m
```

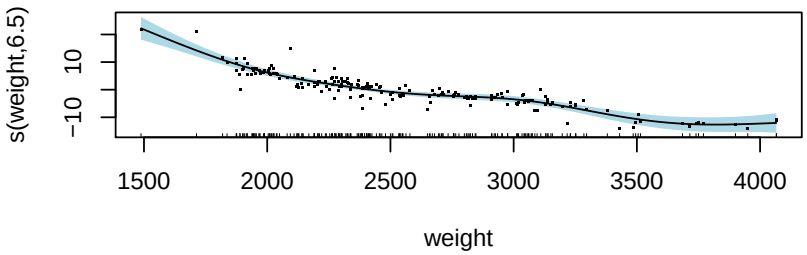
```
plot(gam_mod, pages=1, rug=FALSE)
```

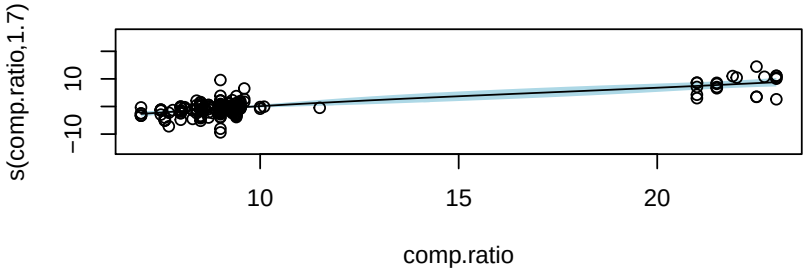


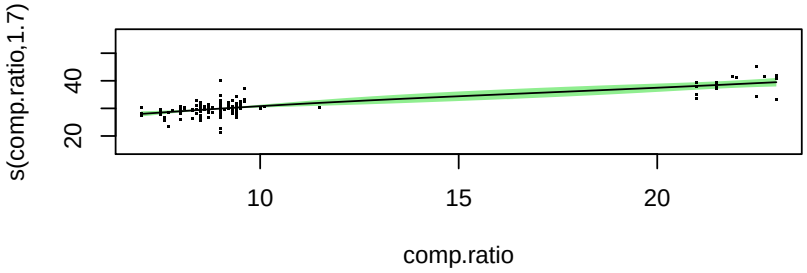

```
par(mfrow=c(2,2))
plot(gam_mod, select = 1, shade = TRUE, residuals = TRUE)
```

```
plot(gam_mod, select = 1, shade = TRUE, residuals = TRUE, shade.col ="lightblue")
plot(gam_mod, select = 4, shade = TRUE, residuals = TRUE, shade.col ="lightblue",
plot(gam_mod, select = 4, shade = TRUE, residuals = TRUE, shade.col ="lightgreen"
```

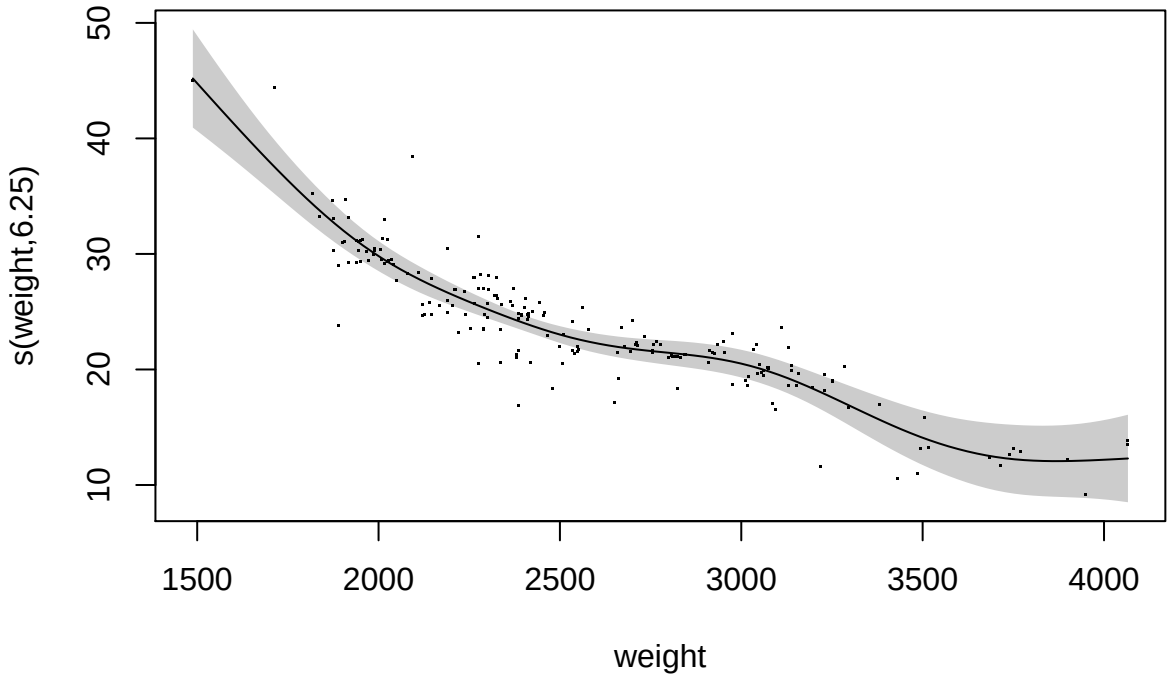








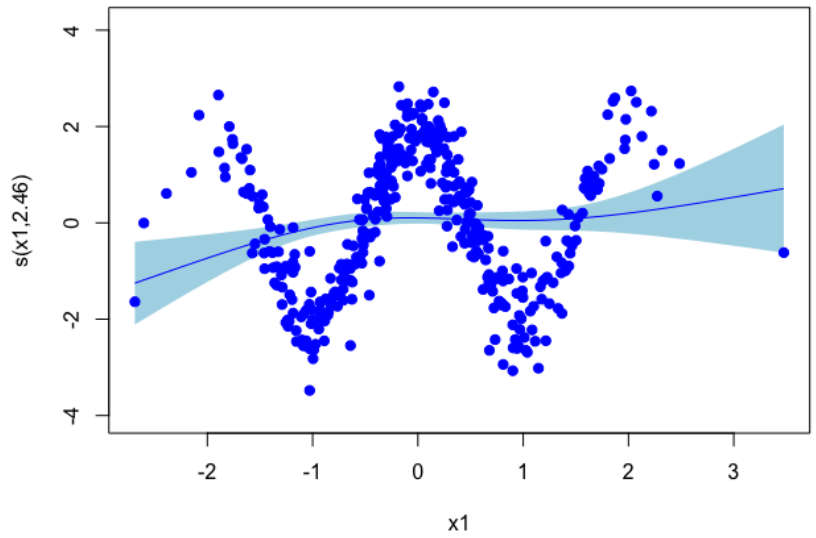

```
plot(mod_city4, select = 1, shade = TRUE, residuals = TRUE, cex=1.2,shift = coef(
```



Model checking, Concurvity

Pitfall One: Inadequate Basis Number

```
mod <- gam(y ~ s(x1, k = 4) + s(x2, k = 4),
           data = check_data, method = "REML")
```



Running gam.check

```
gam.check(mod)
```

```
Method: REML   Optimizer: outer newton
full convergence after 9 iterations.
Gradient range [-0.0001467222,0.00171085]
(score 784.6012 & scale 2.868607).
Hessian positive definite, eigenvalue range [0.00014,198.5]
Model rank =  7 / 7

Basis dimension (k) checking results. Low p-value
(k-index<1) may indicate that k is too low, especially
if edf is close to k'.

        k'  edf k-index p-value
s(x1) 3.00 1.00    0.35  <2e-16 ***
s(x2) 3.00 2.88    1.00    0.52
 ---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
```

Running gam.check (2)

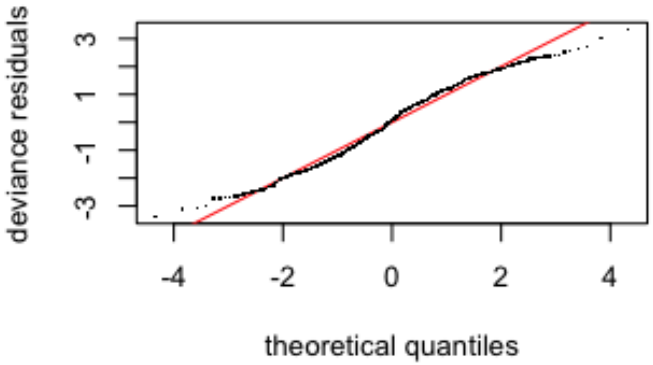
```
mod <- gam(y ~ s(x1, k = 12) + s(x2, k = 4),
           data = dat, method = "REML")
gam.check(mod)
```

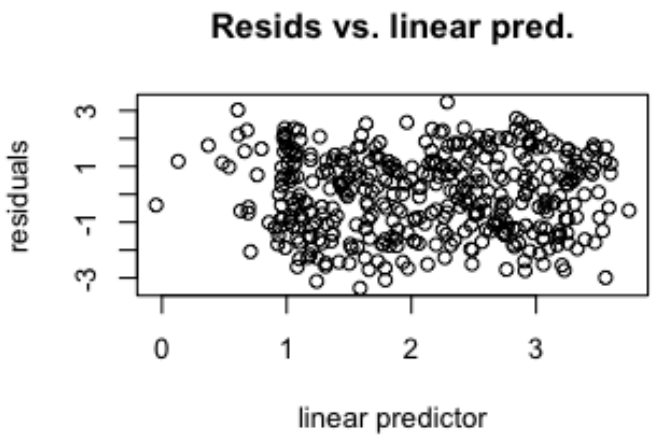
```
...

          k'   edf k-index p-value
s(x1) 11.00 10.85    1.05   0.830
s(x2)  3.00  2.98    0.89   0.015 *

...
```

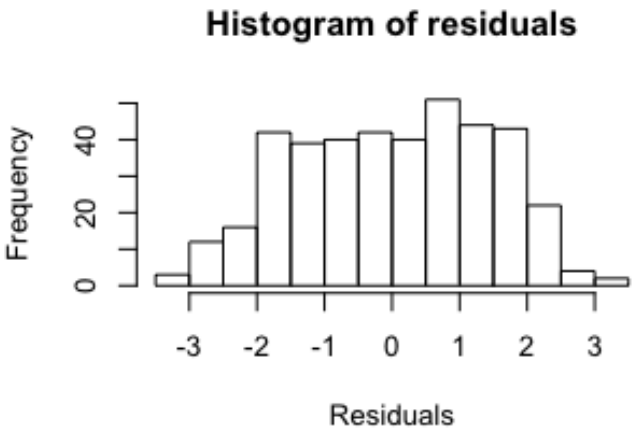
Running gam.check (3)

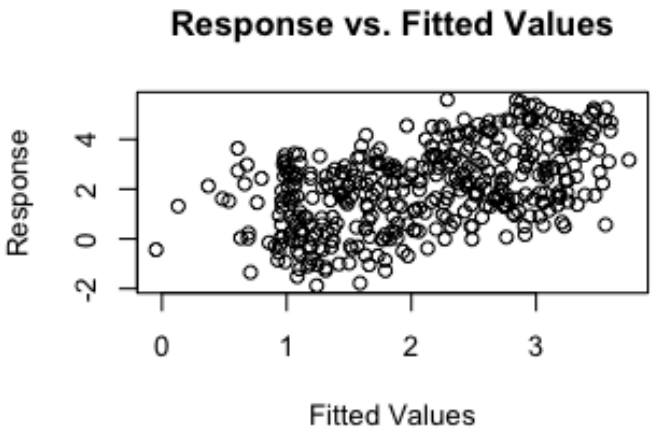
```
mod <- gam(y ~ s(x1, k = 12) + s(x2, k = 12),
           data = dat, method = "REML")
gam.check(mod)
```

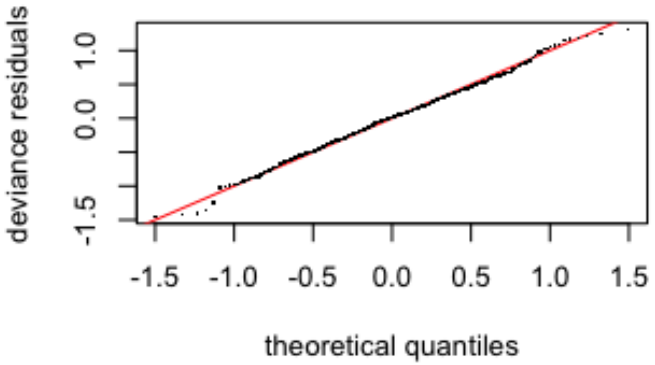
```
...
         k'   edf k-index p-value
s(x1) 11.00 10.86    1.08    0.94
s(x2) 11.00  7.78    0.94    0.12
...
```

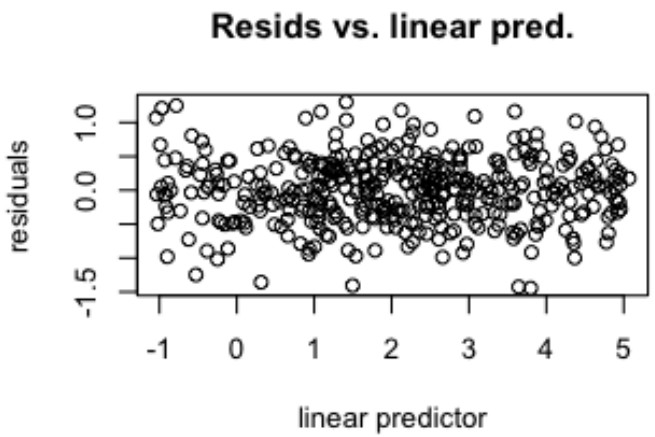

deviance residuals
-3
-1
1
3
-4
-2
0
2
4
theoretical quantiles

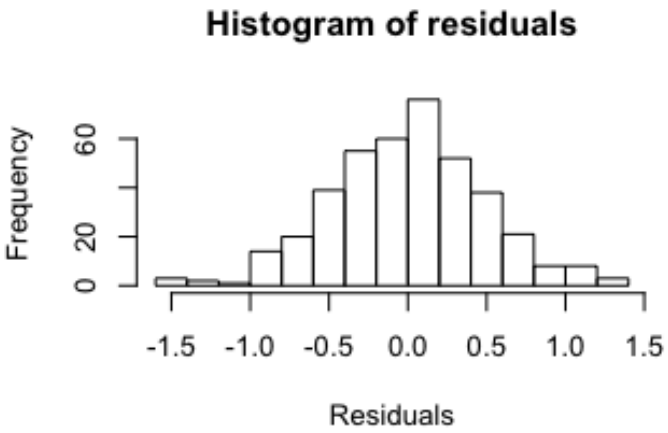

Resids vs. linear pred.
residuals
-3
-1
1
3
0
1
2
3
linear predictor

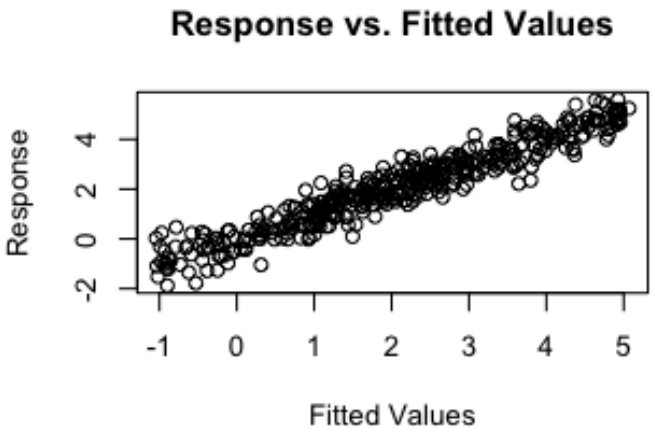

Histogram of residuals
Frequency
0
20
40
-3
-2
-1
0
1
2
3
Residuals

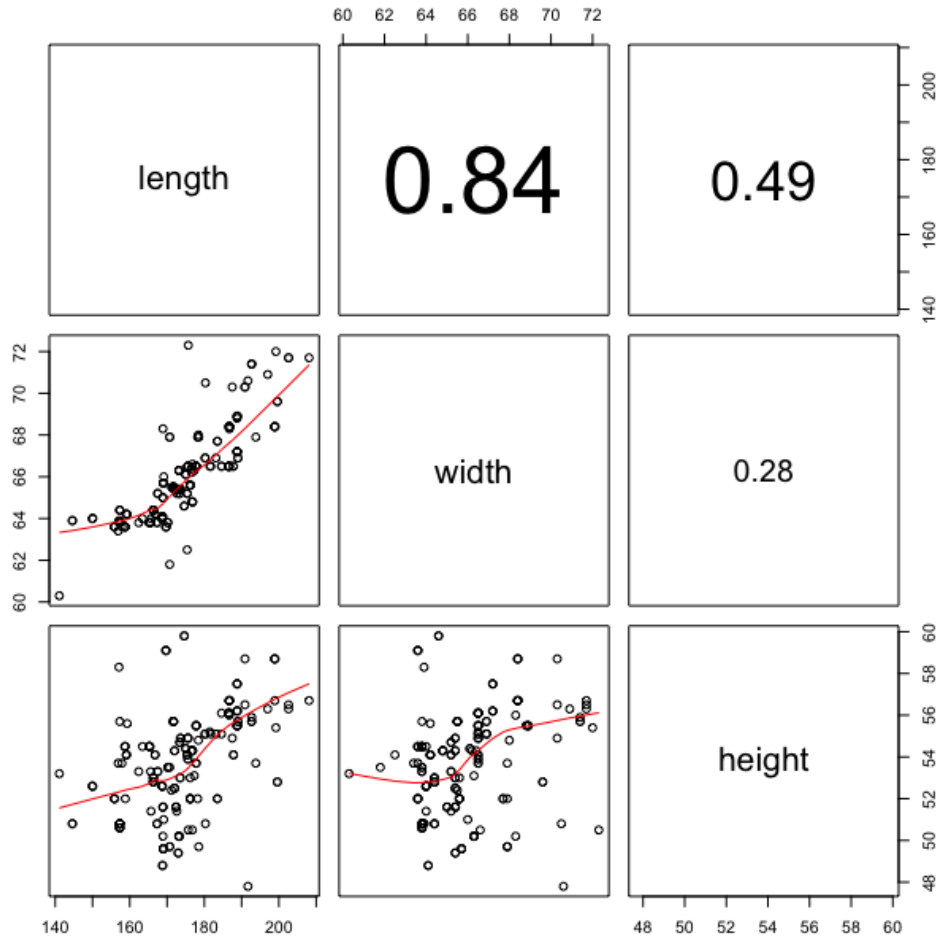

Response vs. Fitted Values
Response
-2
0
2
4
0
1
2
3
Fitted Values


deviance residuals
-1.5
0.0
1.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
theoretical quantiles

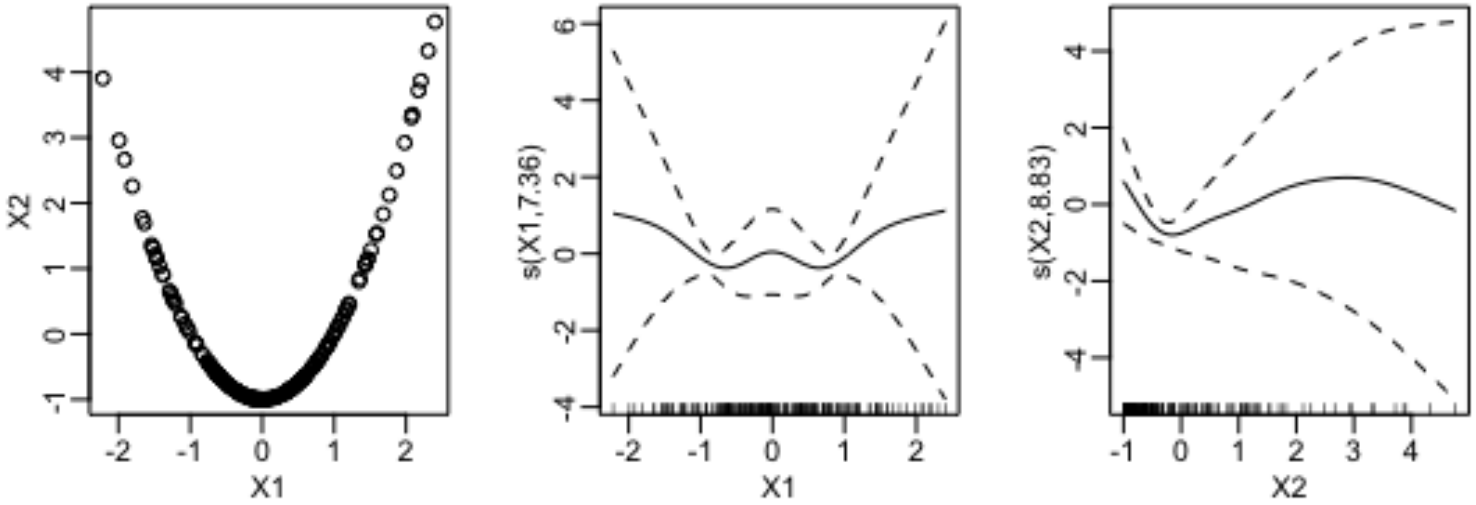

Resids vs. linear pred.
residuals
-1.5
0.0
1.0
-1
0
1
2
3
4
5
linear predictor


Histogram of residuals
Frequency
0
20
60
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Residuals

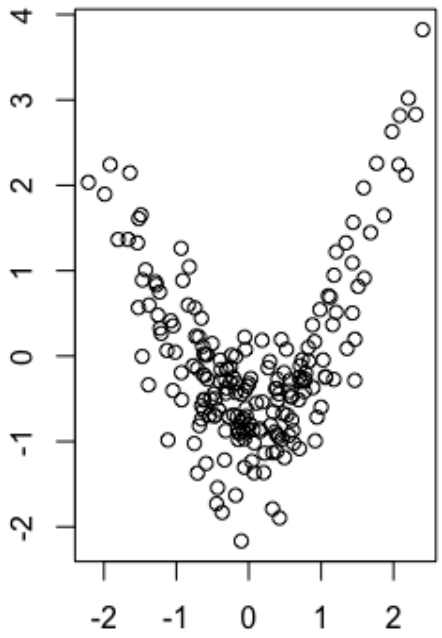

Response vs. Fitted Values
Response
-2
0
2
4
-1
0
1
2
3
4
5
Fitted Values


length
0.84
0.49
width
0.28
height
60 62 64 66 68 70 72
140 160 180 200
48 50 52 54 56 58 60

Concurvity



The concurvity() function




```
concurvity(m1, full = TRUE)
```

```
             para s(X1) s(X2)
worst           0  0.84  0.84
observed        0  0.22  0.57
estimate        0  0.28  0.60
```

Pairwise concurvities

```
concurvity(model, full = FALSE)
```

```
$worst
      para s(X1) s(X2)
para     1  0.00  0.00
s(X1)    0  1.00  0.84
s(X2)    0  0.84  1.00

$observed                    |  $estimate
      para s(X1) s(X2)       |        para s(X1) s(X2)
para     1  0.00  0.00       |  para     1  0.00   0.0
s(X1)    0  1.00  0.57       |  s(X1)    0  1.00   0.6
s(X2)    0  0.22  1.00       |  s(X2)    0  0.28   1.0
```

NONLINEAR MODELING IN R WITH GAMS

Let's practice!

The gam library

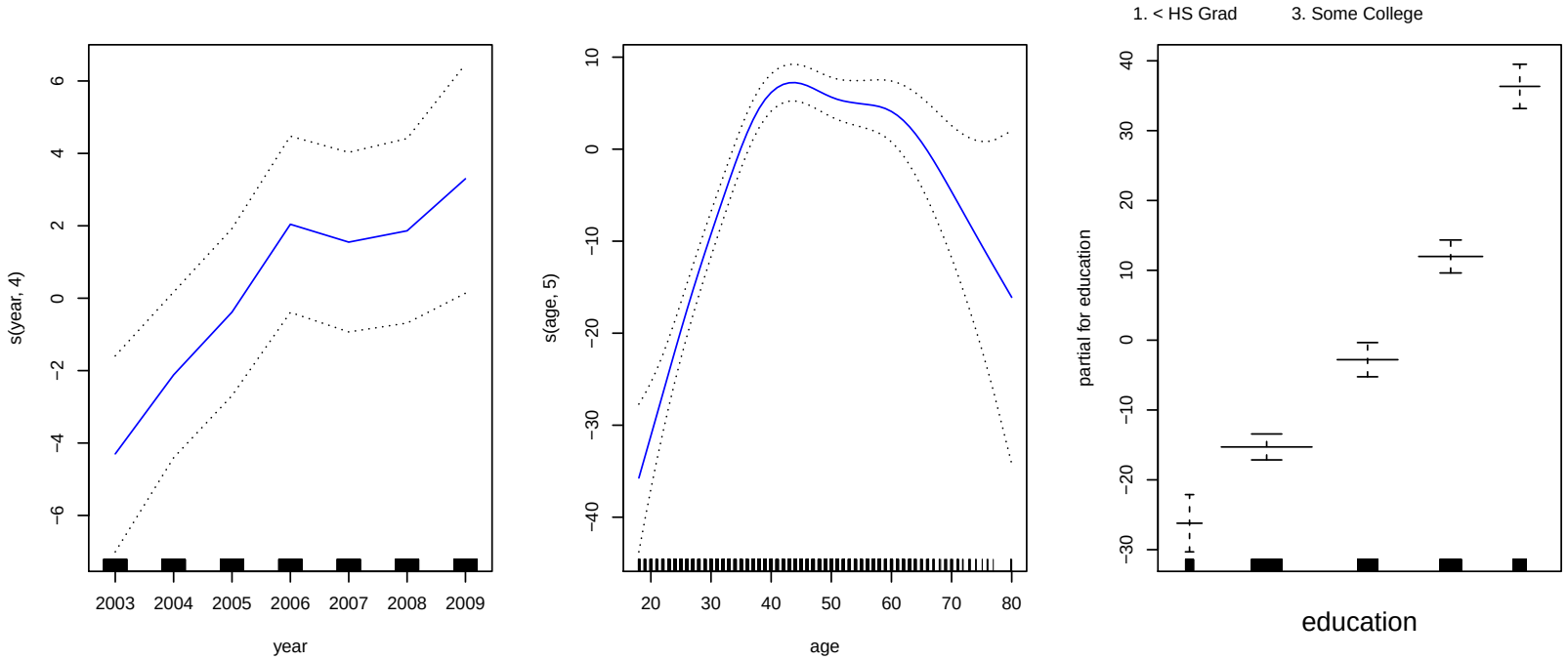
In order to fit more general sorts of GAMs, using smoothing splines or other components that cannot be expressed in terms of basis functions and then fit using least squares regression, we will need to use the gam library in R.

Smoothing/number of knots specified by user

A "simpler" version of mgcv. (no Bayesian smoothing) Note the slightly different syntax though (e.g., df=4, instead of k=4) !!

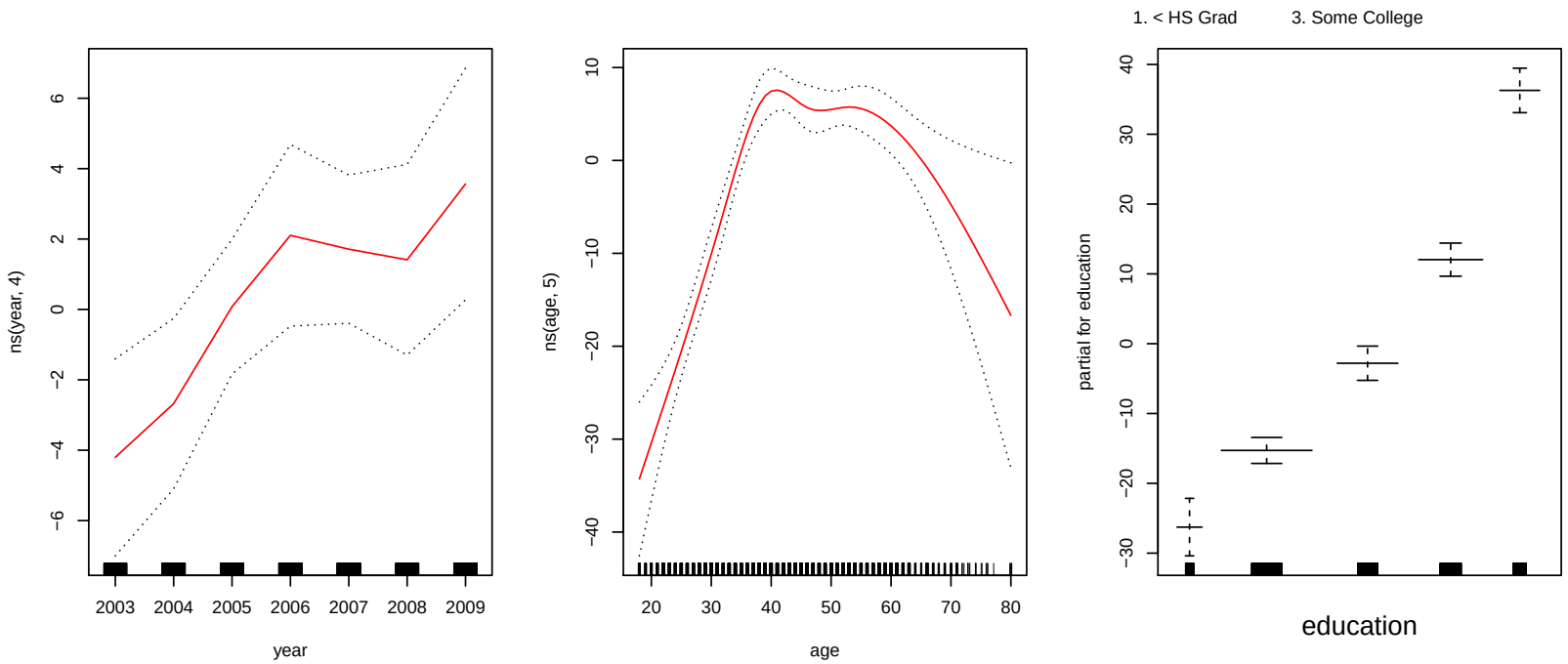
The `s()` function, which is part of the gam library, is used to indicate that we would like to use a smoothing spline. We specify that the function of year should have 4 degrees of freedom, and that the function of *age* will have 5 degrees of freedom. Since *education* is qualitative, we leave it as is, and it is converted into four dummy variables. We use the `gam()` function in order to fit a GAM using these components.

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

detach("package:mgcv", unload=TRUE)#avoid name space collision!
library(gam)
gam.m3 <- gam(wage ~ s(year, 4) + s(age, 5) + education, data = Wage)
par(mfrow = c(1, 3));plot(gam.m3, se = TRUE, col = "blue")
```



Conveniently, even though gam1 is not of class gam but rather of class `lm`, we can still use `plot.gam()` on it.

```
par(mfrow = c(1, 3));plot.Gam(gam1, se = TRUE, col = "red")
```



In these plots, 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).

```
gam.m1 <- gam(wage ~ s(age, 5) + education, data = Wage)
gam.m2 <- gam(wage~ year + s(age, 5) + education, data = Wage)
anova(gam.m1, gam.m2, gam.m3, test = "F")
```

```
## 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       F    Pr(>F)
## 1      2990    3711731
## 2      2989    3693842  1  17889.2 14.4771 0.0001447 ***
## 3      2986    3689770  3   4071.1  1.0982 0.3485661
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We find that there is compelling evidence that a GAM with a linear function of year is better than a GAM that does not include year at all (p-value=0.00014). However, there is no evidence that a non-linear function of year is needed (p-value=0.349). In other words, based on the results of this ANOVA, M2 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:
##     Min      1Q  Median      3Q     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: 2
##
## Anova for Parametric Effects
##              Df  Sum Sq Mean Sq F value    Pr(>F)
## s(year, 4)    1   27162   27162  21.981 2.877e-06 ***
## s(age, 5)     1  195338  195338 158.081 < 2.2e-16 ***
## education     4 1069726  267432 216.423 < 2.2e-16 ***
## 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 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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

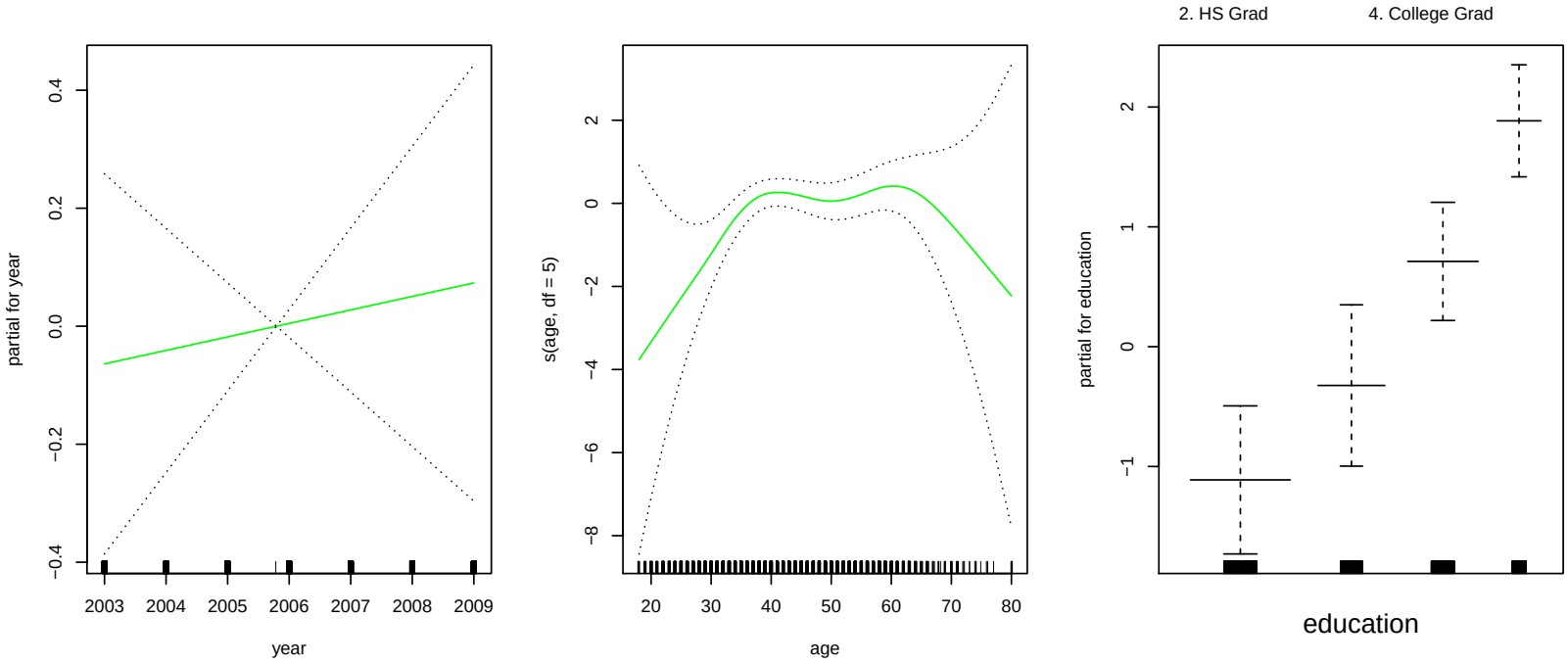
```
preds <- predict(gam.m2, newdata = Wage)
```

Logistic regression

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.s <- gam(I(wage > 250) ~ year + s(age, df = 5) + education,
                family = binomial, data = Wage,
```

```
                    subset = (education != "1. < HS Grad"))
par(mfrow = c(1, 3)); plot(gam.lr.s, se = TRUE, col = "green")
```



Exercises

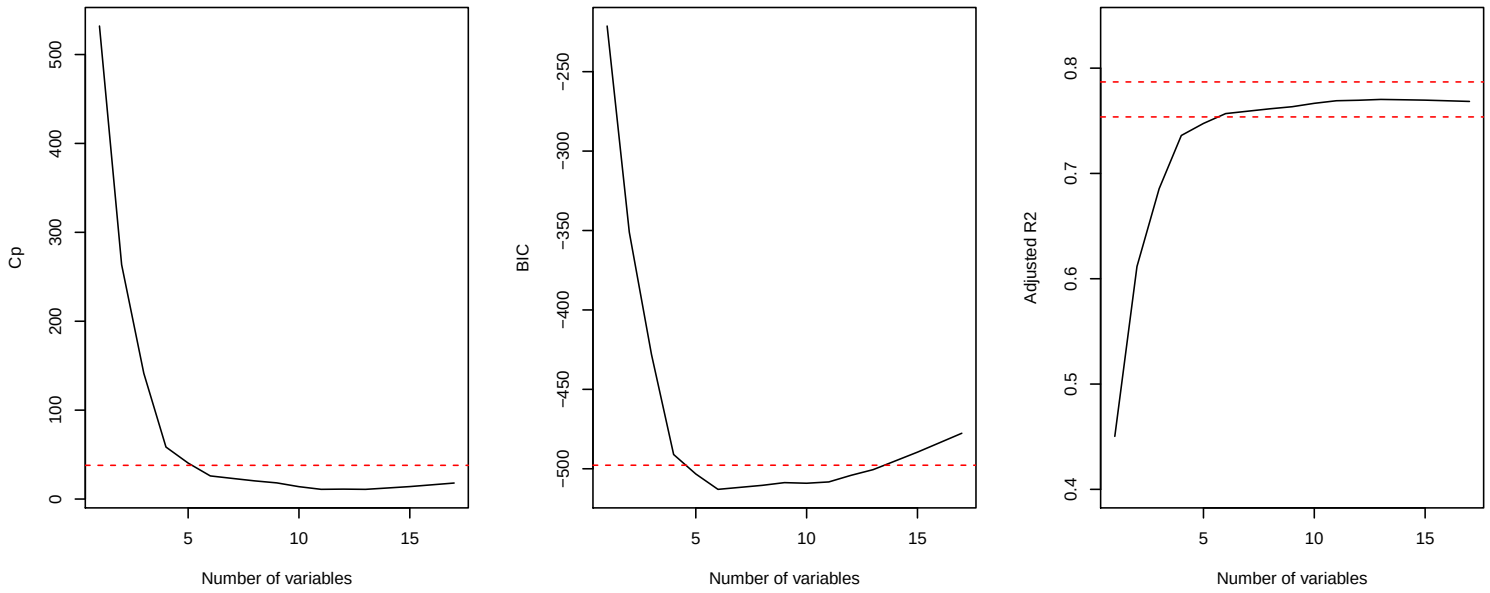
1. **Exercises, Coding**

   This question relates to the "College" data set.

(a) Split the data into a training set and a test set. Using out-of-state tuition as the response and the other variables as the predictors, perform forward stepwise selection on the training set in order to identify a satisfactory model that uses just a subset of the predictors.

```
library(leaps)
set.seed(1)
attach(College)
train <- sample(length(Outstate), length(Outstate) / 2)
test <- -train
College.train <- College[train, ]
College.test <- College[test, ]
fit <- regsubsets(Outstate ~ ., data = College.train, nvmax = 17, method = "
fit.summary <- summary(fit)
par(mfrow = c(1, 3))
plot(fit.summary$cp, xlab = "Number of variables", ylab = "Cp", type = "l")
min.cp <- min(fit.summary$cp)
std.cp <- sd(fit.summary$cp)
abline(h = min.cp + 0.2 * std.cp, col = "red", lty = 2)
abline(h = min.cp - 0.2 * std.cp, col = "red", lty = 2)
plot(fit.summary$bic, xlab = "Number of variables", ylab = "BIC", type='l')
min.bic <- min(fit.summary$bic)
```

```r
std.bic <- sd(fit.summary$bic)
abline(h = min.bic + 0.2 * std.bic, col = "red", lty = 2)
abline(h = min.bic - 0.2 * std.bic, col = "red", lty = 2)
plot(fit.summary$adjr2, xlab = "Number of variables", ylab = "Adjusted R2",
max.adjr2 <- max(fit.summary$adjr2)
std.adjr2 <- sd(fit.summary$adjr2)
abline(h = max.adjr2 + 0.2 * std.adjr2, col = "red", lty = 2)
abline(h = max.adjr2 - 0.2 * std.adjr2, col = "red", lty = 2)
```



Cp, BIC and adjr2 show that size 6 is the minimum size for the subset for which the scores are within 0.2 standard devitations of optimum.

```
fit <- regsubsets(Outstate ~ ., data = College, method = "forward")
coeffs <- coef(fit, id = 6)
names(coeffs)
```

```
## [1] "(Intercept)" "PrivateYes"  "Room.Board"  "PhD"         "perc.alumni"
## [6] "Expend"      "Grad.Rate"
```

(b) Fit a GAM on the training data, using out-of-state tuition as the response and the features selected in the previous step as the predictors. Plot the results, and explain your findings.

(c) Evaluate the model obtained on the test set, and explain the results obtained.

(d) For which variables, if any, is there evidence of a non-linear relationship with the response ?

GAM Exercises part III

Appendix I

Locations of knots

For penalized regression spline, the exact locations are not important, as long as:

- k is adequately big;
- the spread of knots has good, reasonable coverage.

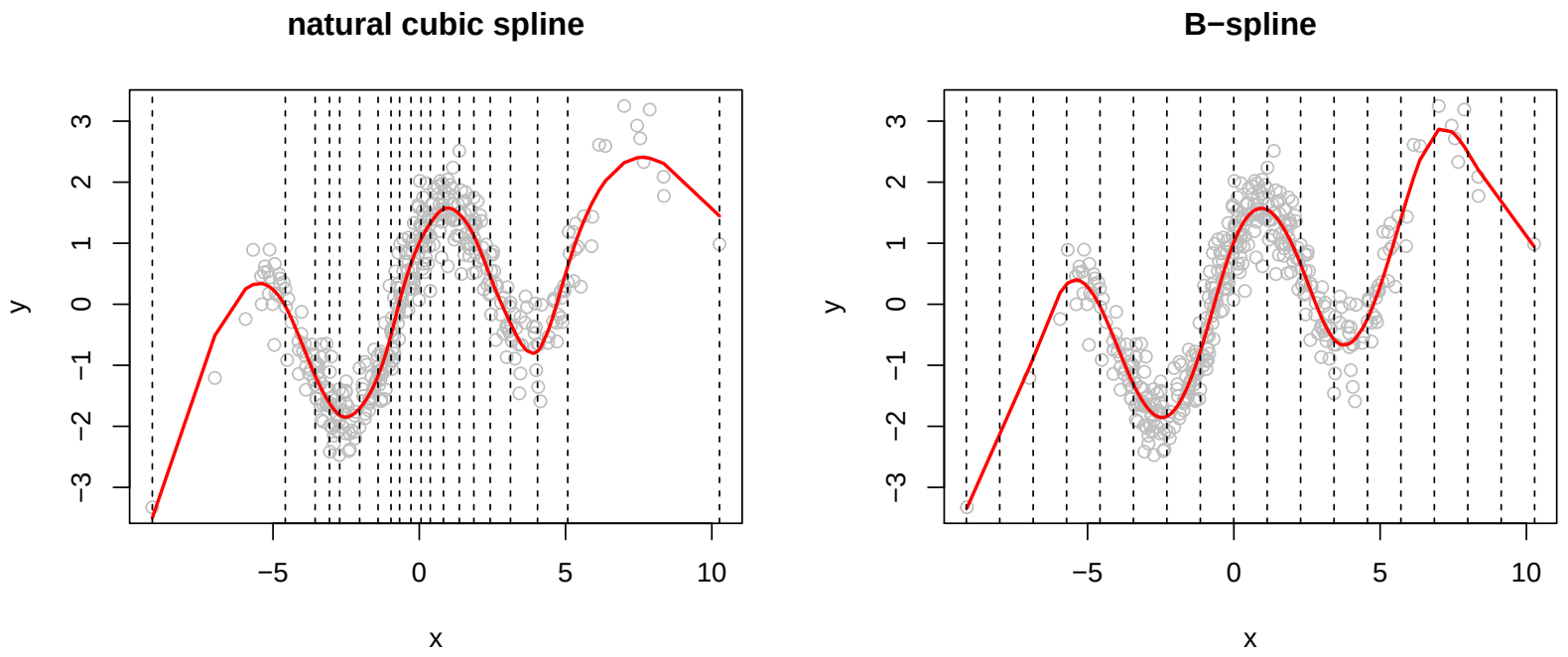
By default:

- natural cubic regression spline bs = 'cr' places knots by quantile;
- B-splines family (bs = 'bs', bs = 'ps', bs = 'ad') place knots evenly.

Compare the following:

```
library(mgcv)

## toy data
set.seed(0); x <- sort(rnorm(400, 0, pi))  ## note, my x are not uniformly sample
set.seed(1); e <- rnorm(400, 0, 0.4)
y0 <- sin(x) + 0.2 * x + cos(abs(x))
y <- y0 + e

## fitting natural cubic spline
```

```r
cr_fit <- gam(y ~ s(x, bs = 'cr', k = 20))
cr_knots <- cr_fit$smooth[[1]]$xp  ## extract knots locations

## fitting B-spline
bs_fit <- gam(y ~ s(x, bs = 'bs', k = 20))
bs_knots <- bs_fit$smooth[[1]]$knots  ## extract knots locations

## summary plot
par(mfrow = c(1,2))
plot(x, y, col= "grey", main = "natural cubic spline");
lines(x, cr_fit$linear.predictors, col = 2, lwd = 2)
abline(v = cr_knots, lty = 2)
plot(x, y, col= "grey", main = "B-spline");
lines(x, bs_fit$linear.predictors, col = 2, lwd = 2)
abline(v = bs_knots, lty = 2)
```



Setting your own knots locations:

You can also provide your customized knots locations via the knots argument of gam() (yes, knots are not fed to s(), but to gam()). For example, you can do evenly spaced knots for cr:

```
xlim <- range(x)  ## get range of x
myfit <- gam(y ~ s(x, bs = 'cr', k =20),
         knots = list(x = seq(xlim[1], xlim[2], length = 20)))
```

Now you can see that:

```
my_knots <- myfit$smooth[[1]]$xp
plot(x, y, col= "grey", main = "my knots");
lines(x, myfit$linear.predictors, col = 2, lwd = 2)
abline(v = my_knots, lty = 2)
```