Splines with Cross-Validation

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First, we need some libraries:

```
library(ISLR2)
```

Next, we look at the included data set:

```
data<-Auto
attach(Auto)
dim(Auto)
```

```
## [1] 392   9
```

We will split the data set into training and validation.

```
#setting the seed for comparable results
set.seed(1)
#first we create the set of indices of what will go into the training set
train <- sample(length(mpg), floor(length(mpg)/2))
#now we put the data with the above indices
#into the training set
training<-data[train,]
dim(training)
```

```
## [1] 196   9
```

```
#the complement of the above indices designates
#the validation set
val<-data[-train,]
dim(val)
```

```
## [1] 196   9
```

Next, we import the library `splines`.

```
library(splines)
```

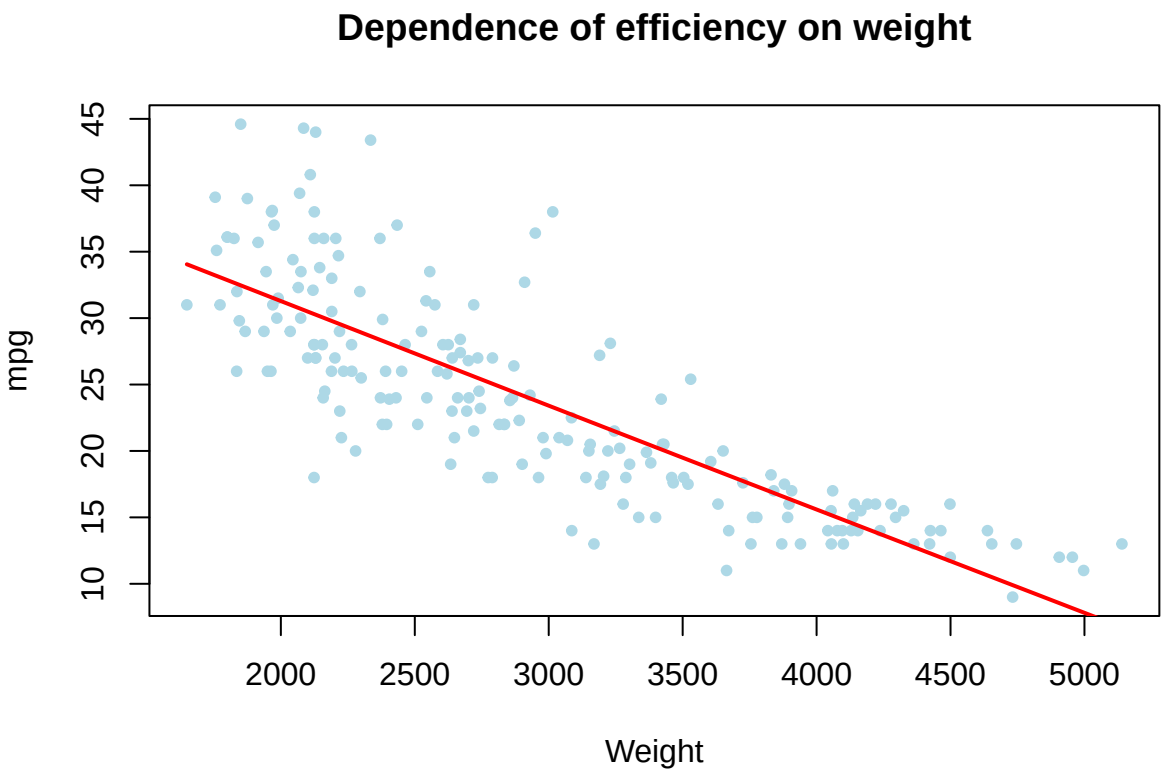
Making a **linear** fit is the same thing as fitting a smooth spline with ....

2 degrees of freedom (corresponding to parameters β_0 and β_1).

```
lin.fit=smooth.spline(training$weight,training$mpg,df=2)
lin.fit
```

```
## Call:
## smooth.spline(x = training$weight, y = training$mpg, df = 2)
##
## Smoothing Parameter  spar= 1.499947  lambda= 16.04335 (30 iterations)
## Equivalent Degrees of Freedom (Df): 2.019589
## Penalized Criterion (RSS): 3827.151
## GCV: 21.48418
```

```r
plot(training$weight,training$mpg,
     col="lightblue", pch=20,
     main="Dependence of efficiency on weight",
     xlab="Weight", ylab="mpg")
lines(lin.fit,col="red", lwd=2)
```




```r
#lm.fit=lm(training$mpg ~ training$weight)
#abline(lm.fit, col="blue")
#what about the fit on the training set?
pred.t<-predict(lin.fit, training$weight)
#what is the structure of `pred.t` here?
pred.t
```

```
## $x
##   [1] 2085 2639 2451 3420 2745 4190 2556 4100 1990 3465 1845 3205 2145 2189 3870
##  [16] 3288 4654 1825 2575 3169 3605 2585 3777 4054 1755 2950 3015 4955 2124 1835
##  [31] 5140 2065 4422 3399 4154 2545 2648 3365 3651 4464 3190 2990 3897 3086 1836
##  [46] 2962 2430 3150 4325 3085 4906 2525 3430 1875 1760 4997 2910 3761 3530 2160
##  [61] 2694 3245 2379 2100 4732 1963 3155 4060 2279 2670 2634 2215 2391 3830 1950
##  [76] 2125 2158 2110 2789 4135 3520 2620 2074 2335 1970 4638 2295 2130 3265 1649
##  [91] 3725 2702 3139 2155 2670 2234 2464 3755 3425 3039
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
##
## $y
##   [1] 30.613641 26.247461 27.728022 20.118214 25.413403 14.112622 26.900928
##   [8] 14.813091 31.362994 19.766286 32.506809 21.801551 30.140402 29.793390
##  [15] 16.604660 21.151326 10.504439 32.664578 26.751312 22.083724 18.672246
##  [22] 26.672573 17.329807 15.171223 33.216772 23.802147 23.291788  8.165163
##  [29] 30.306031 32.585694  6.727539 30.771395 12.308027 20.282493 14.392777
##  [36] 26.987555 26.176622 20.548532 18.313047 11.981457 21.919112 23.488049
```

```
##  [43] 16.394218 22.734627 32.577805 23.707907 27.893491 22.232684 13.062377
##  [50] 22.742472  8.545948 27.145072 20.039996 32.270154 33.177330  7.838780
##  [57] 24.116343 17.454611 19.258183 30.022099 25.814622 21.488130 28.295407
##  [64] 30.495328  9.898196 31.575976 22.193482 15.124505 29.083707 26.003478
##  [71] 26.286817 29.588353 28.200830 16.916494 31.678524 30.298144 30.037873
##  [78] 30.416454 25.067367 14.540653 19.336335 26.397022 30.700405 28.642224
##  [85] 31.520758 10.628803 28.957560 30.258708 21.331461 34.052948 17.735475
##  [92] 25.751677 22.318936 30.061533 26.003478 29.438527 27.625597 17.501417
##  [99] 20.079104 23.103416
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
```

```
pred.t$x
```

```
##   [1] 2085 2639 2451 3420 2745 4190 2556 4100 1990 3465 1845 3205 2145 2189 3870
##  [16] 3288 4654 1825 2575 3169 3605 2585 3777 4054 1755 2950 3015 4955 2124 1835
##  [31] 5140 2065 4422 3399 4154 2545 2648 3365 3651 4464 3190 2990 3897 3086 1836
##  [46] 2962 2430 3150 4325 3085 4906 2525 3430 1875 1760 4997 2910 3761 3530 2160
##  [61] 2694 3245 2379 2100 4732 1963 3155 4060 2279 2670 2634 2215 2391 3830 1950
##  [76] 2125 2158 2110 2789 4135 3520 2620 2074 2335 1970 4638 2295 2130 3265 1649
##  [91] 3725 2702 3139 2155 2670 2234 2464 3755 3425 3039
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
```

```
pred.t$y
```

```
##   [1] 30.613641 26.247461 27.728022 20.118214 25.413403 14.112622 26.900928
##   [8] 14.813091 31.362994 19.766286 32.506809 21.801551 30.140402 29.793390
##  [15] 16.604660 21.151326 10.504439 32.664578 26.751312 22.083724 18.672246
##  [22] 26.672573 17.329807 15.171223 33.216772 23.802147 23.291788  8.165163
##  [29] 30.306031 32.585694  6.727539 30.771395 12.308027 20.282493 14.392777
##  [36] 26.987555 26.176622 20.548532 18.313047 11.981457 21.919112 23.488049
##  [43] 16.394218 22.734627 32.577805 23.707907 27.893491 22.232684 13.062377
##  [50] 22.742472  8.545948 27.145072 20.039996 32.270154 33.177330  7.838780
##  [57] 24.116343 17.454611 19.258183 30.022099 25.814622 21.488130 28.295407
##  [64] 30.495328  9.898196 31.575976 22.193482 15.124505 29.083707 26.003478
##  [71] 26.286817 29.588353 28.200830 16.916494 31.678524 30.298144 30.037873
##  [78] 30.416454 25.067367 14.540653 19.336335 26.397022 30.700405 28.642224
##  [85] 31.520758 10.628803 28.957560 30.258708 21.331461 34.052948 17.735475
##  [92] 25.751677 22.318936 30.061533 26.003478 29.438527 27.625597 17.501417
##  [99] 20.079104 23.103416
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
```

```
#the mean squared error of the predicted values
#in the training set
mean((pred.t$y-training$mpg)^2)
```

```
## [1] 21.04371
```

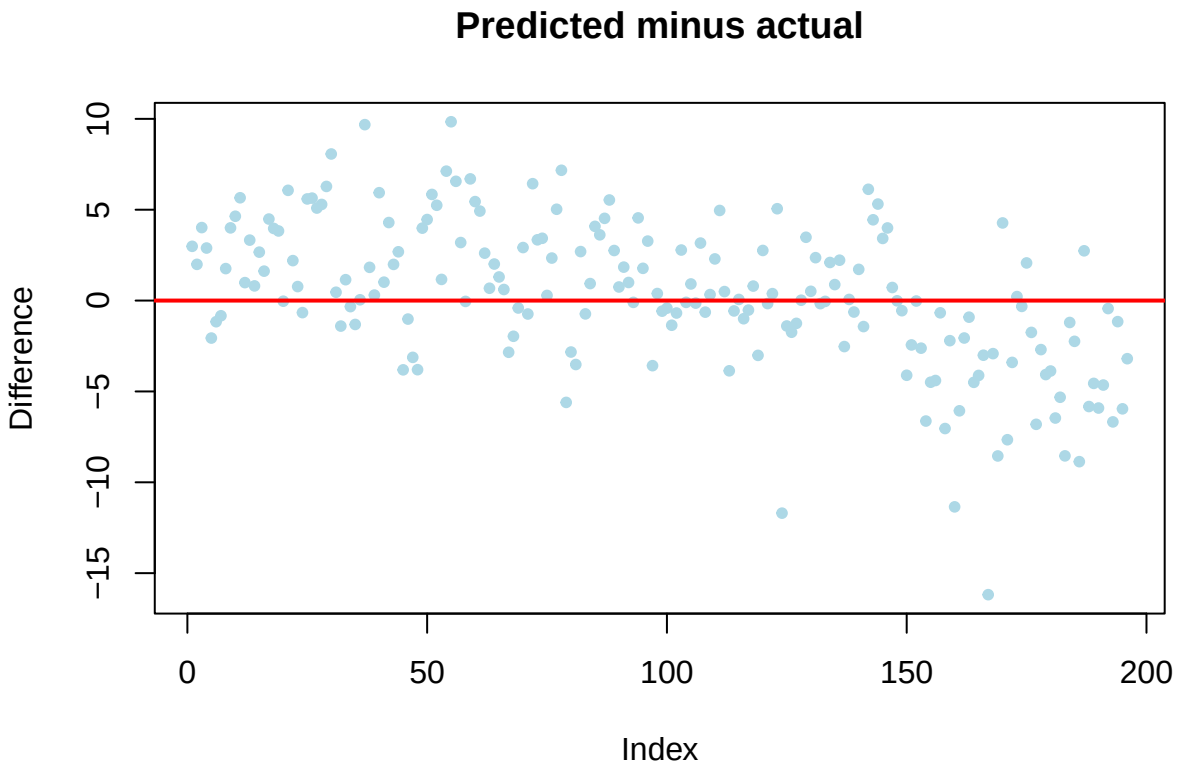
Let's see how this fit performs on the validation set.

```
pred <- predict(lin.fit, val$weight)
#what does `predict` give us in this case?
pred
```

```
## $x
##   [1] 3693 3436 3433 3449 4341 4354 4312 3850 3563 3609 2587 2672 2375 4615 4376
##  [16] 4382 2228 3439 3329 4209 2408 3282 2065 1613 1834 1955 2278 2126 2254 2408
##  [31] 4274 4385 3672 4633 4502 4456 2330 4098 4294 2933 2288 2506 2164 3988 4952
```

```
##  [46] 4464 4735 4951 3821 3121 2945 3021 2904 2401 2310 2472 2265 4082 2582 2868
##  [61] 2807 3102 1950 2542 3781 3613 4699 4457 4257 2300 2003 2108 2246 2489 2000
##  [76] 3264 3432 3158 4668 4440 4657 3730 3785 2171 2914 2592 2223 2984 3211 2957
##  [91] 2945 2671 1795 2220 2572 2255 4215 3962 4215 3233
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
##
## $y
##   [1] 17.985195 19.993069 20.016532 19.891401 12.937934 12.836829 13.163491
##   [8] 16.760566 19.000327 18.641006 26.656826 25.987739 28.326933 10.807581
##  [15] 12.665736 12.619076 29.485839 19.969606 20.830307 13.964779 28.066856
##  [22] 21.198314 30.771395 34.336932 32.593582 31.639082 29.091591 30.290257
##  [29] 29.280823 28.066856 13.459079 12.595746 18.149108 10.667667 11.686015
##  [36] 12.043659 28.681639 14.828661 13.303502 23.935669 29.012749 27.294728
##  [43] 29.990553 15.685213  8.188476 11.981457  9.874880  8.196247 16.986668
##  [50] 22.460093 23.841416 23.244692 24.163481 28.122020 28.839304 27.562569
##  [57] 29.194090 14.953220 26.696194 24.446353 24.925838 22.609116 31.678524
##  [64] 27.011182 17.298608 18.609767 10.154677 12.035884 13.591328 28.918141
##  [71] 31.260448 30.432228 29.343903 27.428643 31.284112 21.339294 20.024353
##  [78] 22.169961 10.395622 12.168065 10.481121 17.696462 17.267410 29.935346
##  [85] 24.084919 26.617458 29.525267 23.535157 21.754530 23.747173 23.841416
##  [92] 25.995609 32.901233 29.548924 26.774935 29.272938 13.918094 15.887747
##  [99] 13.918094 21.582145
##  [ reached 'max' / getOption("max.print") -- omitted 96 entries ]
```

```r
#plot of how "off" the predictions are
plot(pred$y-val$mpg,
     col="lightblue", pch=20,
     main="Predicted minus actual",
     xlab="Index", ylab="Difference")
abline(0,0, col="red", lwd=2)
```



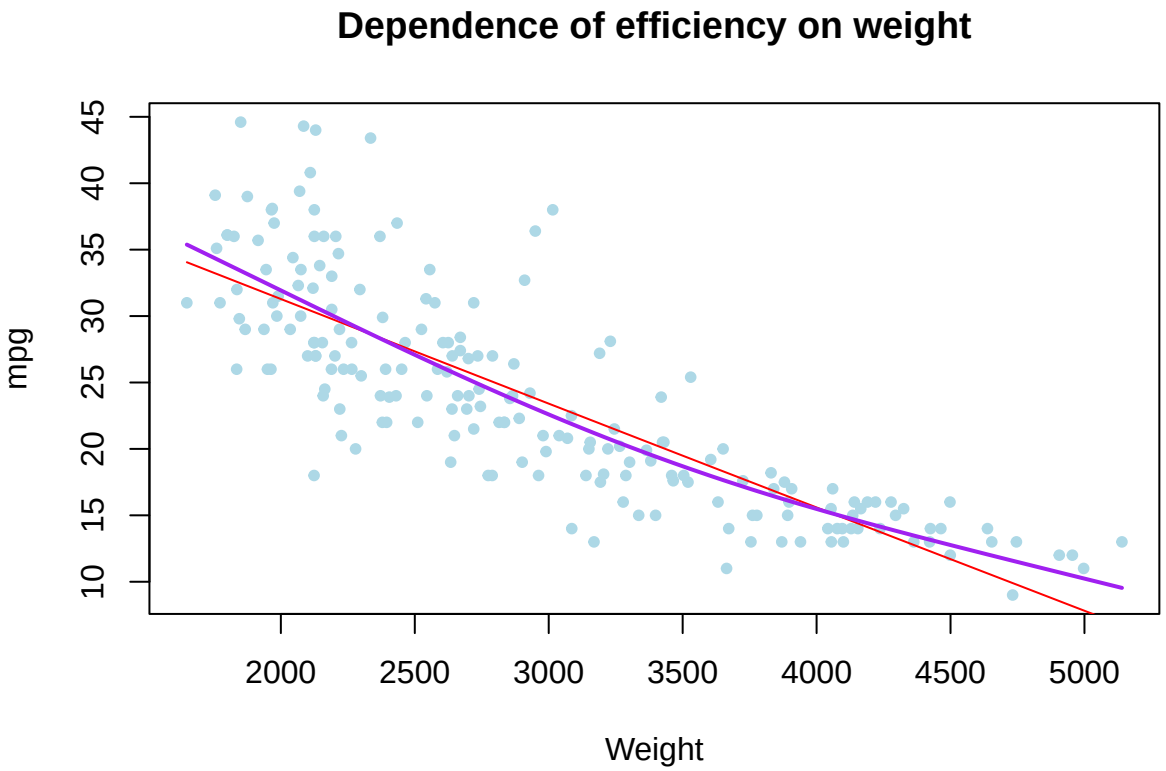
```r
#the mean squared error of the predicted values
#on the validation set
mean((pred$y-val$mpg)^2)
```

```
## [1] 16.32753
```

How would the **quadratic** fit work? That's what we get with 3 degrees of freedom.

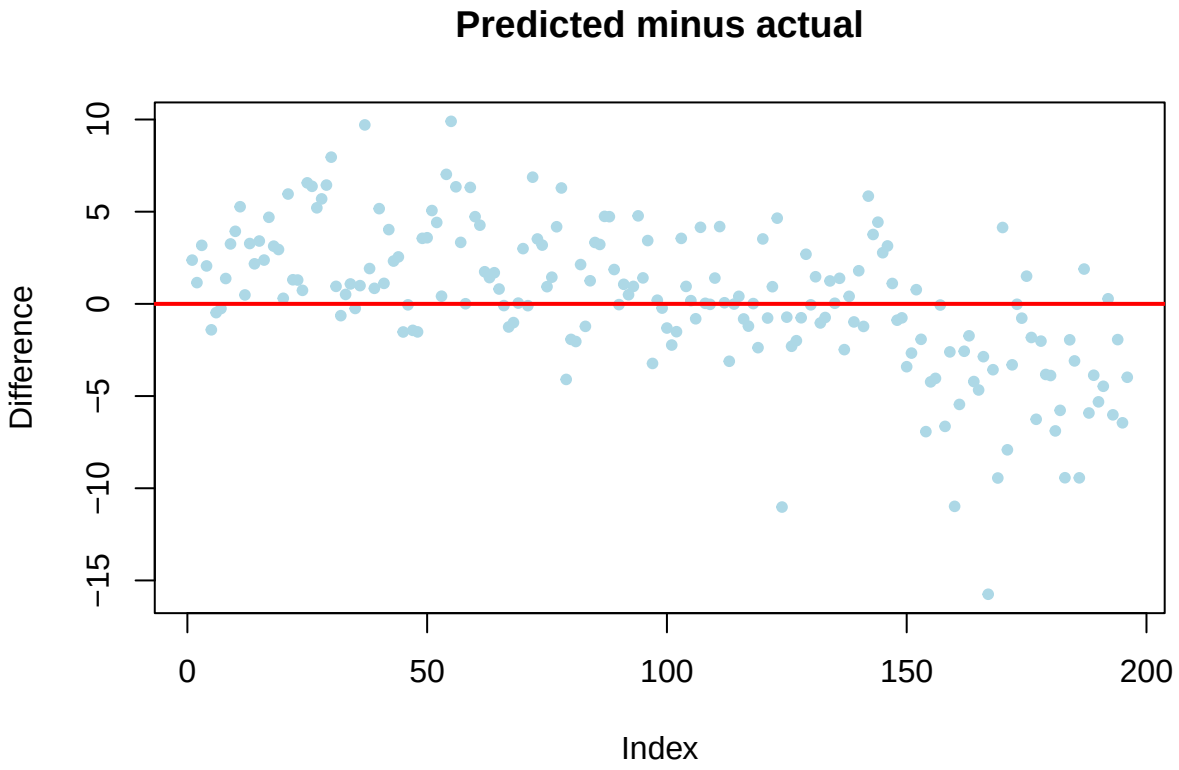
```r
q.fit=smooth.spline(training$weight,training$mpg,df=3)

plot(training$weight,training$mpg,
     col="lightblue", pch=20,
     main="Dependence of efficiency on weight",
     xlab="Weight", ylab="mpg")
lines(lin.fit, col="red")
lines(q.fit,col="purple", lwd=2)
```



How well did we do on the validation set?

```r
#as before, we create the predicted values
pred <- predict(q.fit, val$weight)
#plot of how "off" the predictions are
plot(pred$y-val$mpg,
     col="lightblue", pch=20,
     main="Predicted minus actual",
     xlab="Index", ylab="Difference")
abline(0,0, col="red", lwd=2)
```




```
#the mean squared error of the predicted values
#in the validation set
mean((pred$y-val$mpg)^2)
```

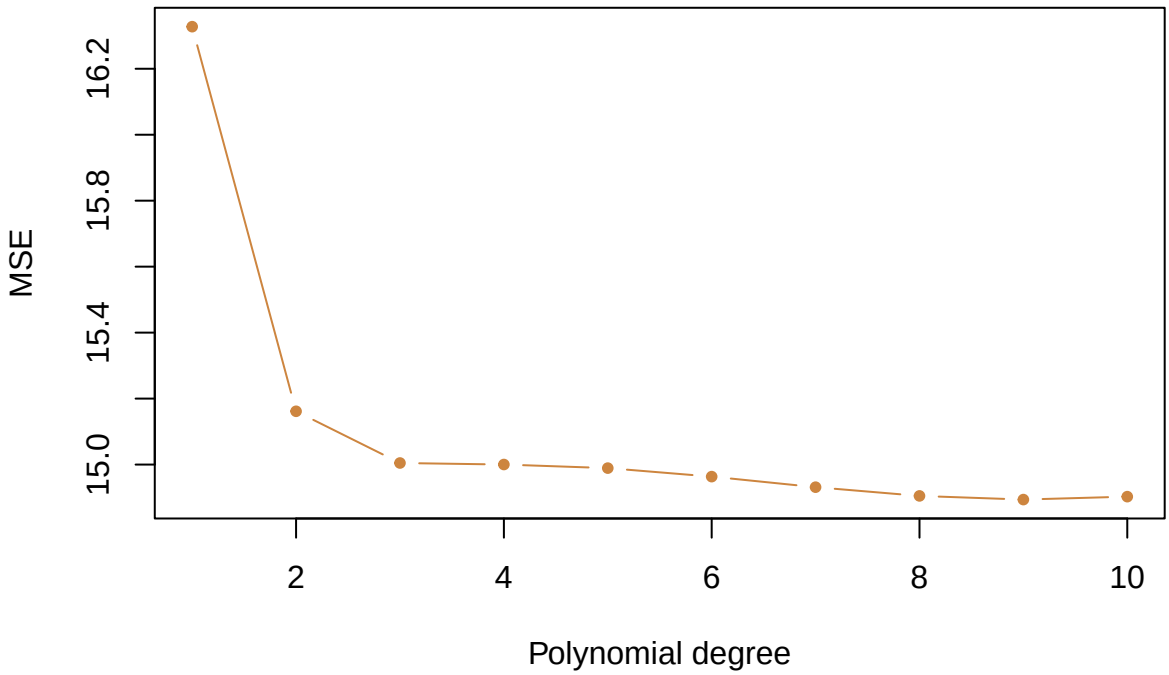
```
## [1] 15.1615
```

It might be fun to go through a `for` loop and see what the MSEs on the validation set are as we increase the number of degrees of freedom.

```
#first we choose the maximal number of degrees of freedom
max.deg=10
#now, we create a numeric vector which will contain
#validation set MSEs
MSEs=numeric(max.deg)
#next, we repeat the procedures we had before `max.deg` times
for (deg in 1:max.deg){
  fit=smooth.spline(training$weight,training$mpg,df=deg+1)
  pred <- predict(fit, val$weight)
  MSEs[deg]=mean((pred$y-val$mpg)^2)
}
print(MSEs)
```

```
##  [1] 16.32753 15.16150 15.00475 15.00011 14.98925 14.96347 14.93146 14.90495
##  [9] 14.89386 14.90271
```

```
#let's plot the MSEs as they depend
#on the degree of the polynomial
plot(MSEs, type="b",
     xlab="Polynomial degree",
     ylab="MSE",
     col="peru", pch=20)
```



What would we get if we let R optimize the number of degrees of freedom using LOOCV?

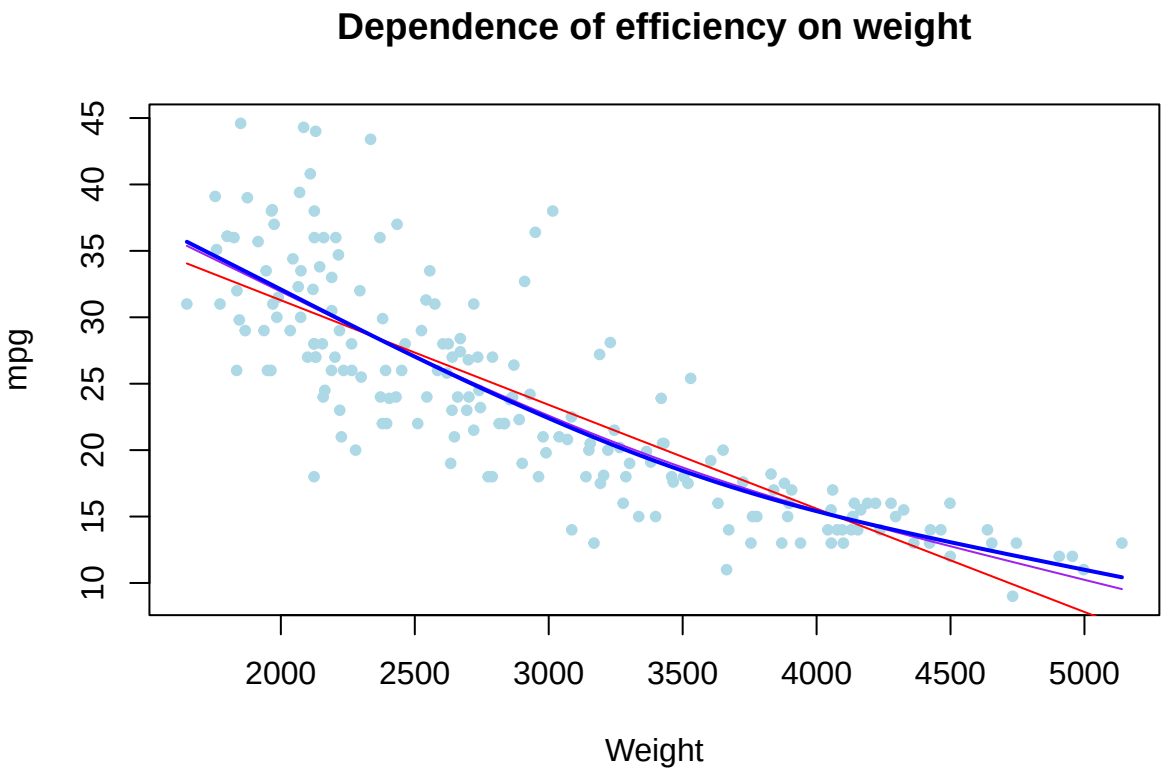
```
fit.cv=smooth.spline(training$weight,training$mpg,cv=T)
```

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

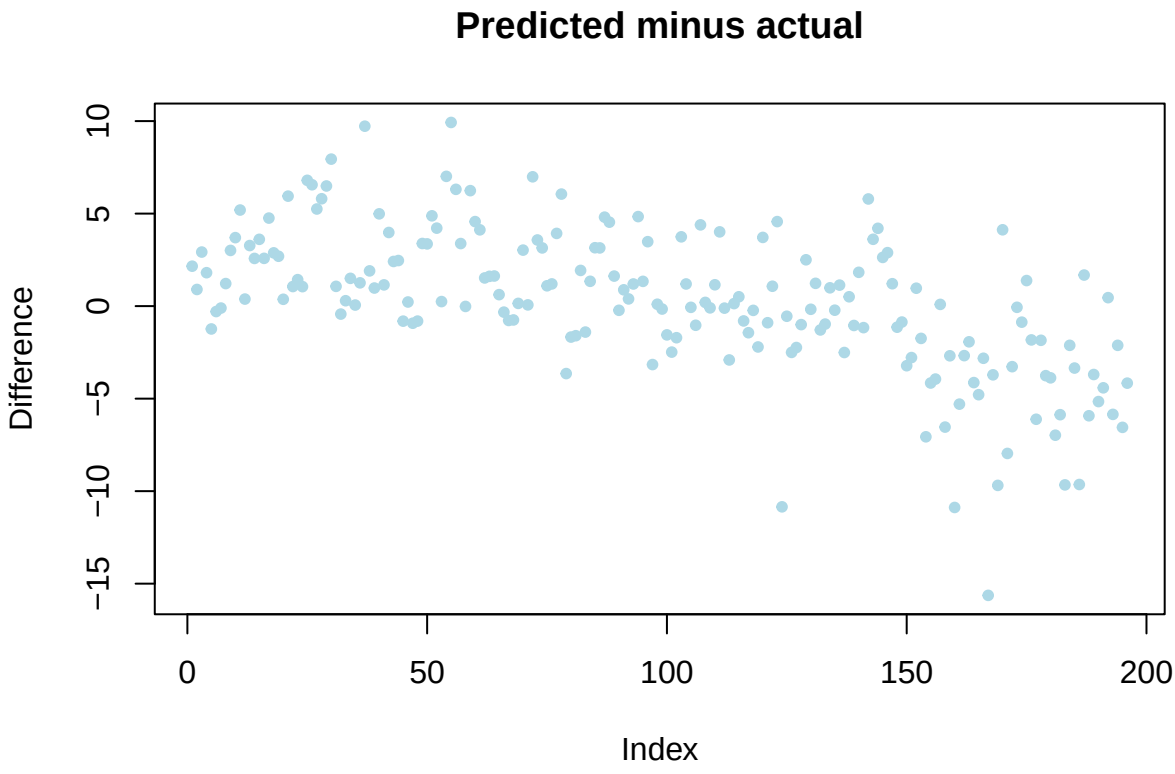
```
#summary(fit.cv)
fit.cv$df
```

```
## [1] 3.548739
```

```
plot(training$weight,training$mpg,
     col="lightblue", pch=20,
     main="Dependence of efficiency on weight",
     xlab="Weight", ylab="mpg")
lines(lin.fit, col="red")
lines(q.fit,col="purple")
lines(fit.cv,col="blue",lwd=2)
```




```
pred <- predict(fit.cv, val$weight)
plot(pred$y-val$mpg, pch=20, col="lightblue",
     xlab="Index", ylab="Difference",
     main="Predicted minus actual")
```



```r
mean((pred$y-val$mpg)^2)
```

```
## [1] 15.02952
```