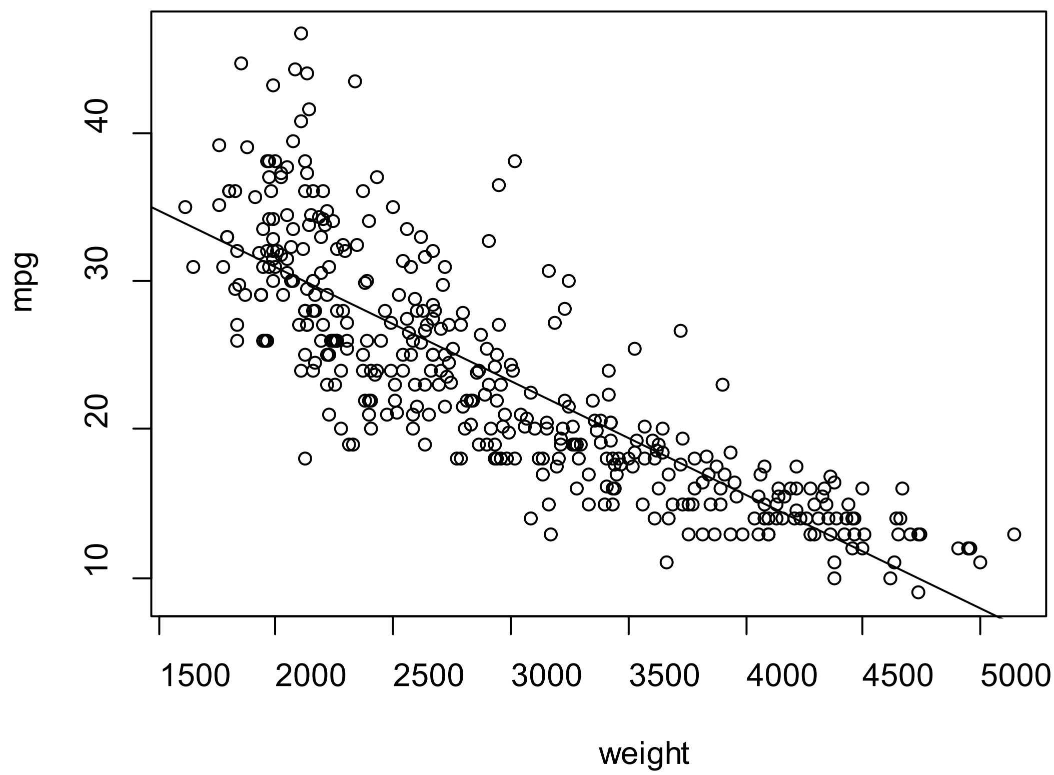
POLYNOMIALS AND SPLINES

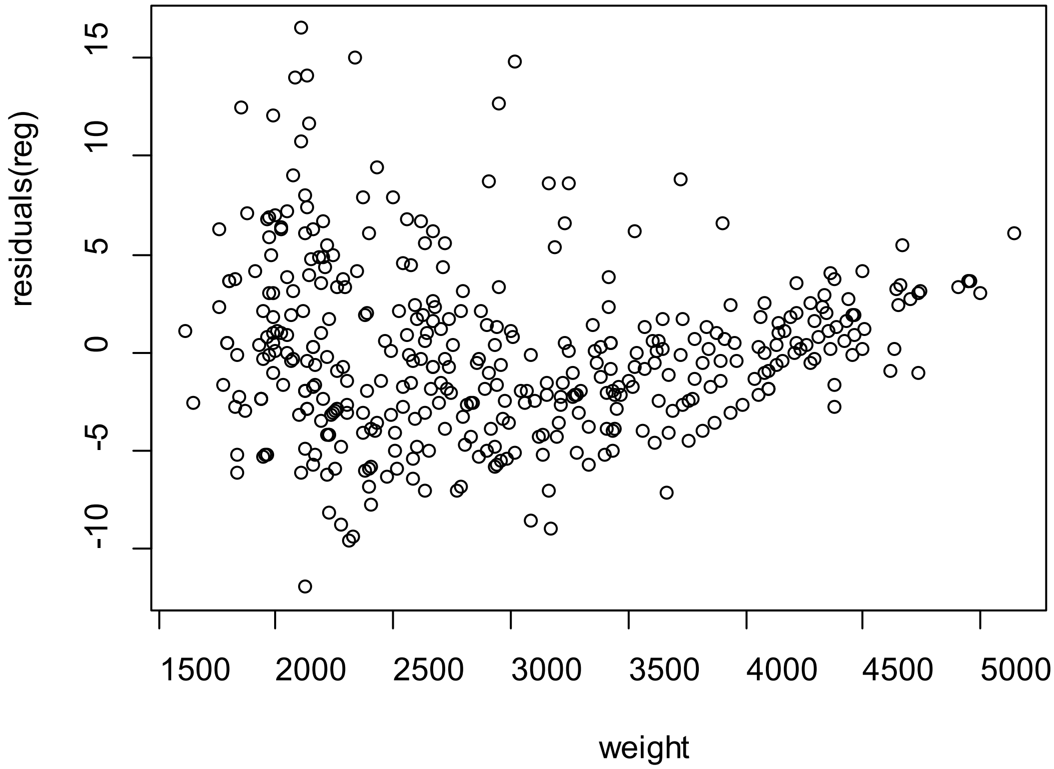
1. Fitting a polynomial regression

```
> attach(Auto);
> plot( weight, mpg )
> reg = lm( mpg ~ weight )
> abline(reg)
```



 # Look at the residuals. Is linear model adequate?

```
> plot( weight, residuals(reg) )
```



 # If a polynomial regression is appropriate, what is the best degree?

> install.packages("leaps")

> library(leaps)

> polynomial.fit = regsubsets(mpg ~ poly(weight,10), data=Auto)

> summary(polynomial.fit)

```
poly(weight, 10)1 poly(weight, 10)2 poly(weight, 10)3 poly(weight, 10)4 poly(weight, 10)5
poly(weight, 10)6
1  ( 1 ) "*"               " "               " "               " "               " "
" "
2  ( 1 ) "*"               "*"               " "               " "               " "
" "
3  ( 1 ) "*"               "*"               " "               " "               " "
" "
4  ( 1 ) "*"               "*"               " "               " "               " "
" "
5  ( 1 ) "*"               "*"               " "               " "               "*"
" "
6  ( 1 ) "*"               "*"               " "               " "               "*"
"*"
7  ( 1 ) "*"               "*"               " "               " "               "*"
"*"
8  ( 1 ) "*"               "*"               " "               "*"               "*"
"*"
         poly(weight, 10)7 poly(weight, 10)8 poly(weight, 10)9 poly(weight, 10)10
1  ( 1 ) " "               " "               " "               " "
2  ( 1 ) " "               " "               " "               " "
3  ( 1 ) " "               " "               " "               "*"
4  ( 1 ) "*"               " "               " "               "*"
5  ( 1 ) "*"               " "               " "               "*"
6  ( 1 ) "*"               " "               " "               "*"
7  ( 1 ) "*"               " "               "*"               "*"
8  ( 1 ) "*"               " "               "*"               "*"
```

> which.max(summary(polynomial.fit)$adjr2)

[1] 4

> which.min(summary(polynomial.fit)$cp)

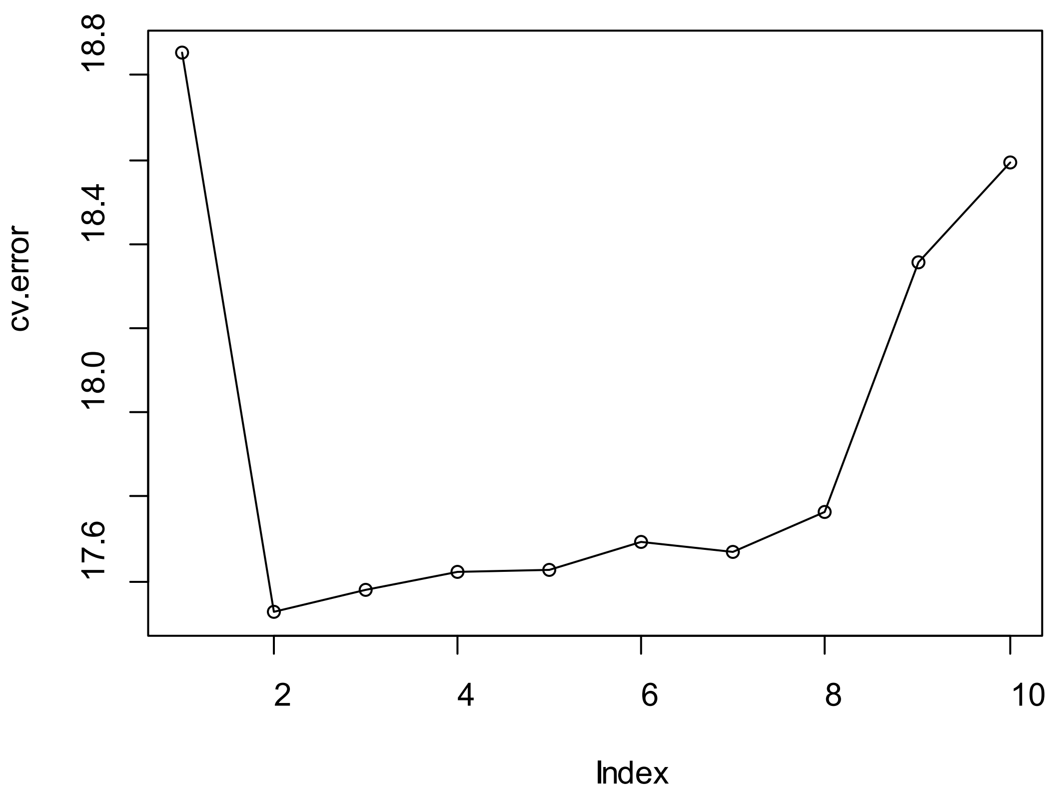
[1] 3

> which.min(summary(polynomial.fit)$bic)
[1] 2

 # BIC chooses a quadratic model "*mpg =* $\beta_0 + \beta_1$ *(weight) +* β_2*(weight)*^{2} *+ ε*". Mallows C_p and adjusted R^2 add higher order terms.

 # Cross-validation agrees with the quadratic model…

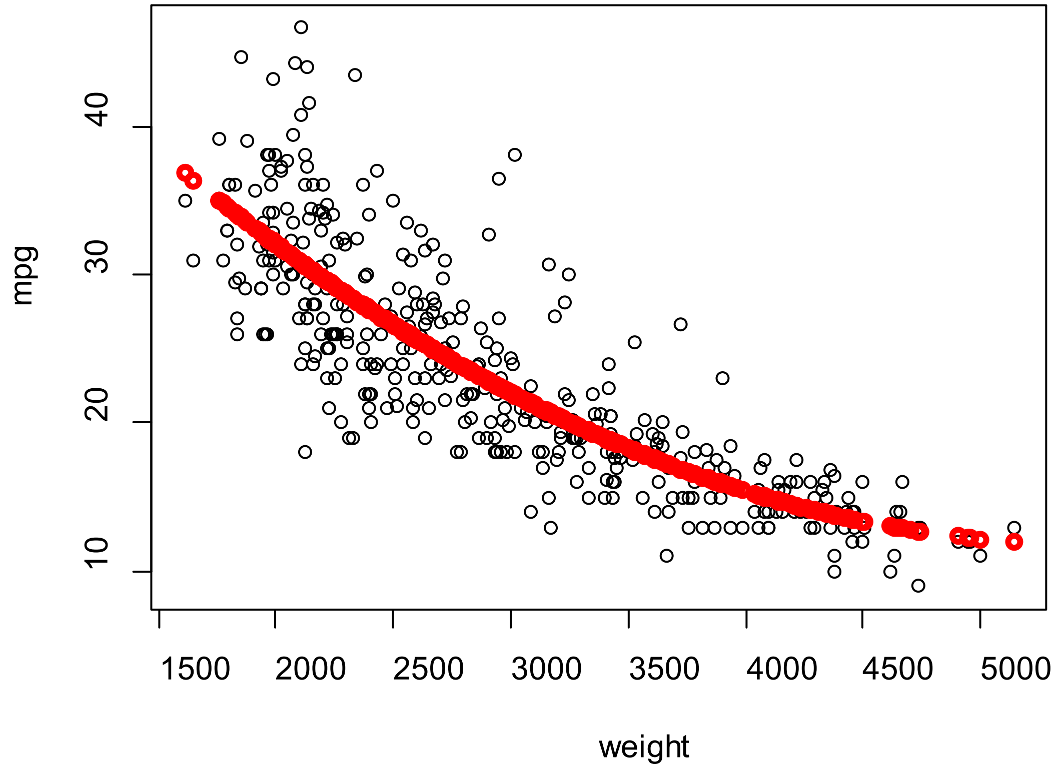
```
> library(boot)
> cv.error = rep(0,10)
> for (p in 1:10){
+ polynomial = glm( mpg ~ poly(weight,p) )
+ cv.error[p] = cv.glm( Auto, polynomial )$delta[1] }
> cv.error
 [1] 18.85161 17.52474 17.57811 17.62324 17.62822 17.69418 17.66695 17.76456 18.35543 18.59401
> plot(cv.error); lines(cv.error)
```



 # So, we choose the quadratic regression – degree 2 polynomial. Its prediction MSE is 17.52.

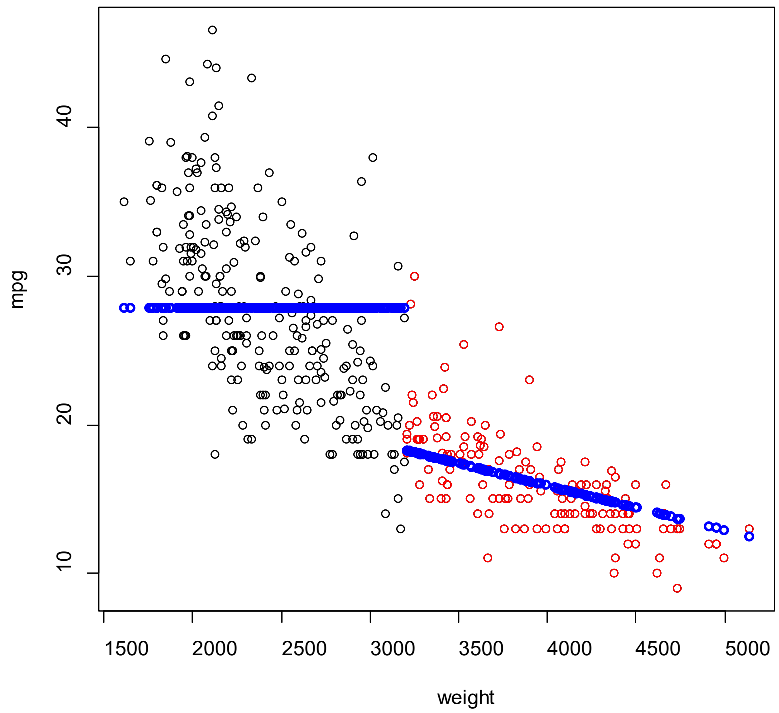
```
> poly2 = lm( mpg ~ poly(weight,2) )
> summary(poly2)
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)    
(Intercept)          23.4459     0.2109 111.151  < 2e-16 ***
poly(weight, 2)1   -128.4436     4.1763 -30.755  < 2e-16 ***
poly(weight, 2)2     23.1589     4.1763   5.545 5.43e-08 ***

> plot( weight,mpg )
> Yhat_poly2 = fitted.values( poly2 )
```

> points(weight, Yhat_poly2, col="red", lwd=3)



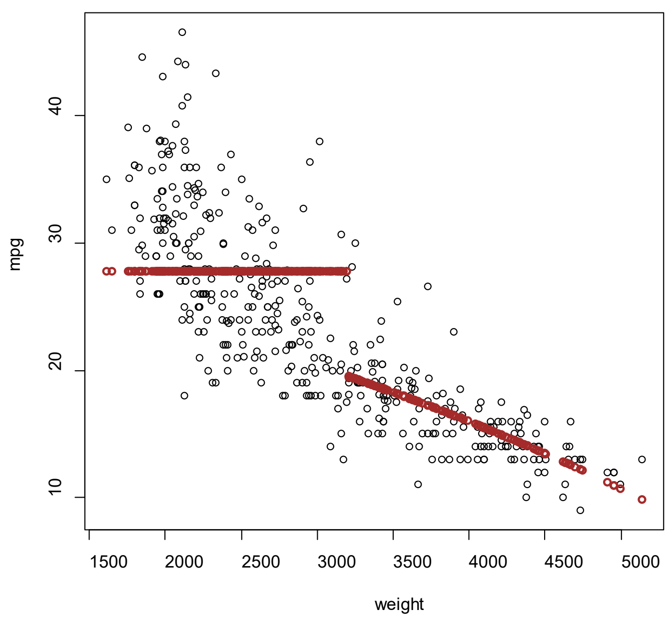
<u>2. Broken Line</u> – fitting different models on different intervals of X.

```
> n = length(mpg);                              # From the residual plot, the trend
> Group = 1*(weight > 3200)                     # changes around weight = 3200 lbs
> plot(weight, mpg, col = Group+1 )             # Red points correspond to heavier cars
> broken_line = lm( mpg ~ weight : Group )      # Interactions allow different slopes
> Yhat_broken = predict(broken_line)            # Fitted values
> points( weight, Yhat_broken, lwd=2, col="blue" )  # Add fitted values to the plot
```



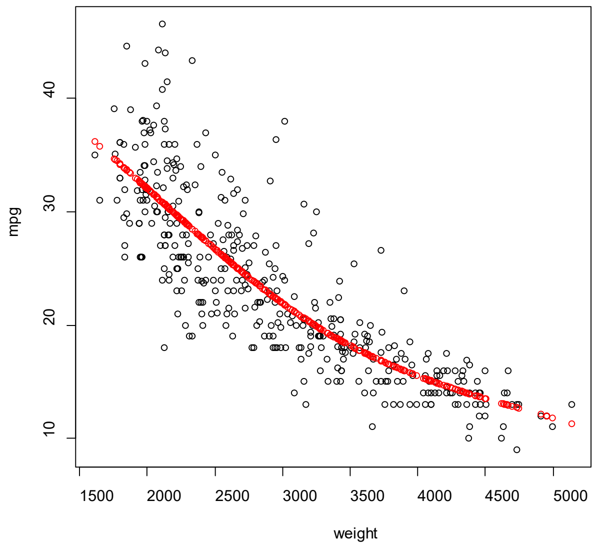
 # Quadratic polynomial fit does not improve the picture

> broken_quadratic = lm(mpg ~ (weight + I(weight^2)) : Group)
> Yhat_broken_quadratic = predict(broken_quadratic)
> plot(weight,mpg);   points(weight, Yhat_broken, lwd=2, col="brown")



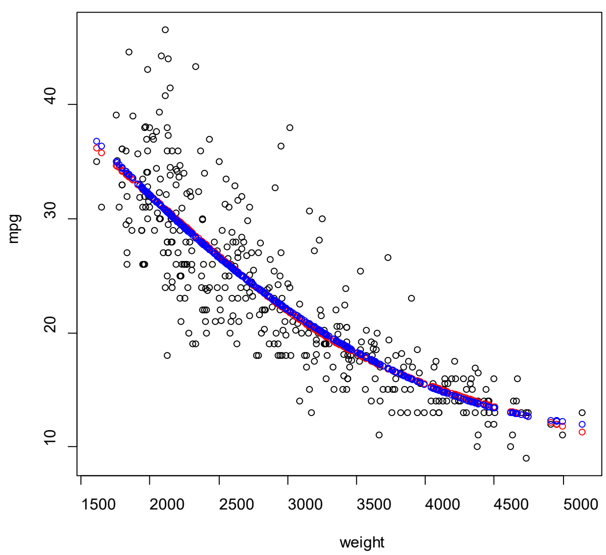
<u>3. Splines</u> – smooth connection at knots.

> install.packages("splines")
> library(splines)
> spline = lm(mpg ~ bs(weight, knots=3200))   **# In this lm, we defined the basis and knots**
> Yhat_spline = predict(spline)   **# Fitted values**
> plot(weight,mpg);   points(weight, Yhat_spline, col="red")



 # This spline is almost the same as the quadratic polynomial regression!

> points(weight, Yhat_poly2, col="blue")

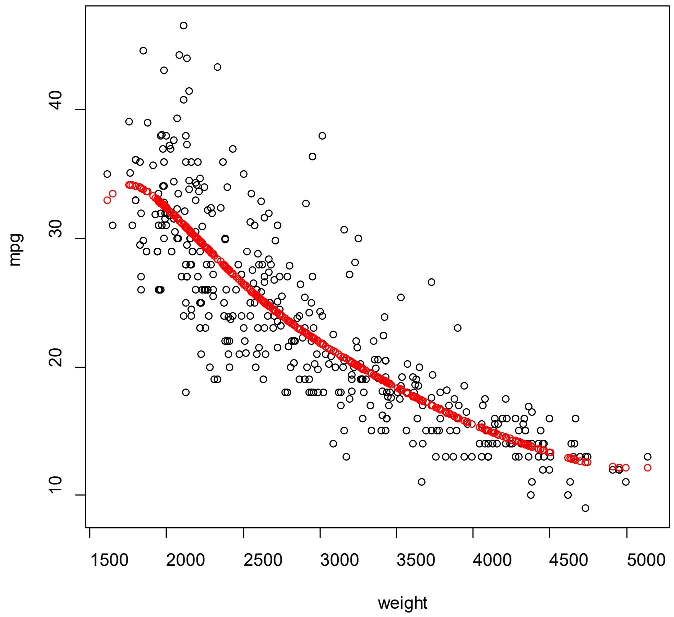


 # Add more knots?

> spline = lm(mpg ~ bs(weight, knots=c(2000,2500,3200,4500)))

> Yhat_spline = predict(spline)

> plot(weight,mpg);   points(weight, Yhat_spline, col="red")



4. Cross-validation

> library(boot)

 # Compare these four models by K-fold cross-validation, with K=n/4 groups, deleting 4 units at a time.

```
> reg = glm( mpg ~ weight )
> poly2 = glm( mpg ~ poly(weight,2) )
> spline1knot = glm( mpg ~ bs(weight, knots=3200) )
> spline4knots = glm( mpg ~ bs(weight, knots=c(2000,2500,3200,4500)) )

> cv.glm( Auto, reg, K=n/4 )$delta[1]
[1] 18.84014
> cv.glm( Auto, poly2, K=n/4 )$delta[1]
[1] 17.51702
> cv.glm( Auto, spline1knot, K=n/4 )$delta[1]
[1] 17.59429
> cv.glm( Auto, spline4knots, K=n/4 )$delta[1]
[1] 17.81641
```

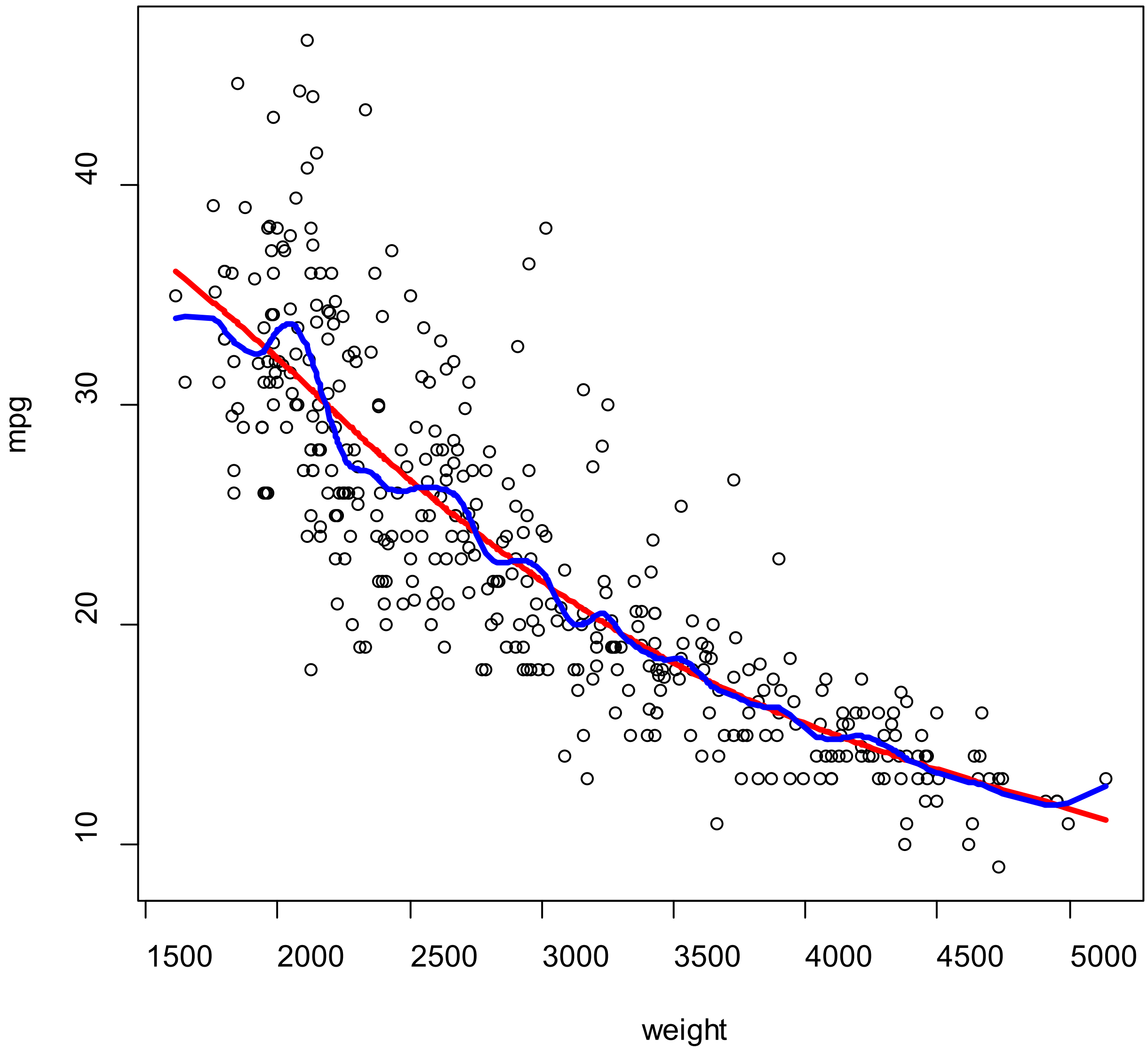
 # The quadratic polynomial model wins. Splitting X range into segments for the splints did not make much difference.

5. Smoothing Splines

5a. Fitting a smoothing spline

```
> attach(Auto);     plot(weight,mpg);     attach(splines);
> ss5 = smooth.spline(weight, mpg, df=5)
> lines(ss5, col="red", lwd=3)
```

> ss25 = smooth.spline(weight, mpg, df=25)
> lines(ss25, col="blue", lwd=3)



 # A spline with (an equivalent of) 5 degrees of freedom is very smooth, its flexibility is limited by small df. A spline with 25 df is probably too flexible, too wiggly. The optimal df can be determined by cross-validation.

5b. Prediction error and cross-validation

> n = length(mpg);   Z = sample(n,200);   attach(Auto[Z,]);   **# This will be training data of size 200 (for example)**
> ss5 = smooth.spline(weight, mpg, df=5)   **# Fit the spline using training data only**

> attach(Auto);
> Yhat = predict(ss,x=weight)
> names(Yhat)   **# Notice: prediction consists of two parts – predictor x and**
[1] "x" "y"   **# predicted response y. We can call them as Yhat$x and Yhat$y.**

> mean((Yhat$y[-Z] - mpg[-Z])^2) **# Then, compute prediction mean-squared error on test data**
[1] 16.58982 **# This is the cross-validation error for a spline with df=5**

R also has a built-in cross-validation tool for smoothing splines. It uses the leave-one-out method (LOOCV, or jackknife)

> smooth.spline(weight, mpg, df=5, cv=TRUE)

Smoothing Parameter spar= 1.046238 lambda= 0.01789013 (11 iterations)
Equivalent Degrees of Freedom (Df): 5.000653
Penalized Criterion: 5974.815
PRESS: 17.59263 **# This error (PREdiction Sum of Squares) is computed by LOOCV method**

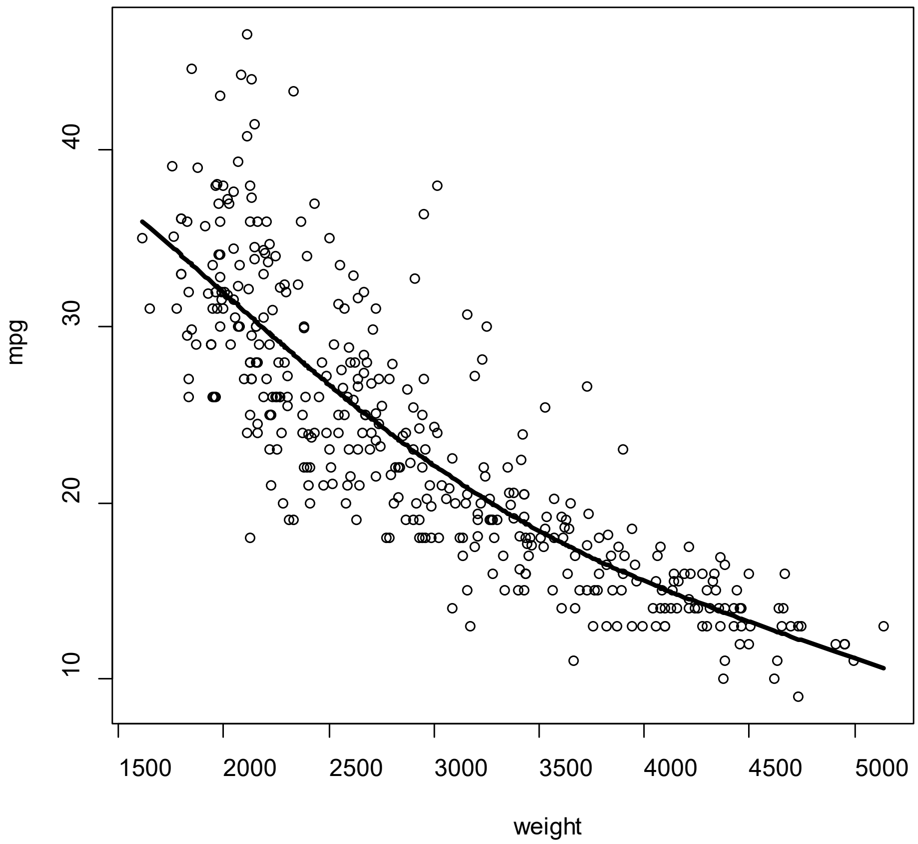
5c. Choosing the optimal degrees of freedom

We'll fit smoothing splines of various df and choose the one with the smallest prediction error.

```
> cv.err = rep(0,50);    Auto.train = Auto[Z,];
> for (p in 1:50){
+ attach(Auto.train);  ss = smooth.spline(weight, mpg, df=p+0.01)           # DF should be > 1
+ attach(Auto);      Yhat = predict(ss, weight)
+ cv.err[p] = mean( (Yhat$y[-Z] - mpg[-Z])^2 ) }

> which.min(cv.err)
[1] 1
```

 # This cross-validation chooses the smoothing spline with the equivalent of df=1.01

```
> ss = smooth.spline(weight, mpg, df=1.01)
> Yhat = predict(ss)
> plot(weight,mpg); lines(Yhat, lwd=3)
```


mpg
10
20
30
40
weight
1500
2000
2500
3000
3500
4000
4500
5000