ZZCS8506 — Regression analysis for data Scientists

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Based on the notes provided by Boris Beranger

Deparment of Statistics

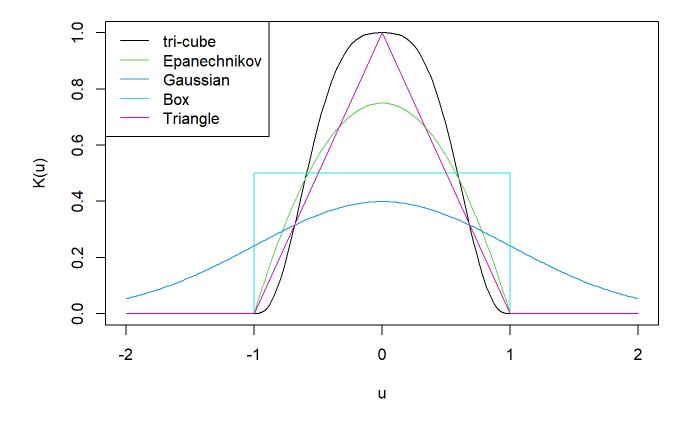
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5.1. Loess Smoother

Different kinds of weighting functions

Below, we visualise some weighting functions that can be used in the loess algorithm. Note that they all integrate to 1. They mathematical definition is provided in the teaching materilas.

```
xx1=seq(from = -1, to = 1, length.out = 100)
# tri-cube Kernel
yy=(1-abs(xx1)^3)^3
plot(xx1,yy,xlim = c(-2,2),type='l',xlab='u',ylab='K(u)'); lines(x=c(-2,-1),y=c(0,
0)); lines(c(1,2),c(0,0))
# Epanechikov kernel
yy=3/4*(1-xx1^2)
lines(xx1,yy,col=3)
xx2=seq(from = -2, to = 2, length.out = 200)
# Gaussian kernel
yy=dnorm(xx2)
lines(xx2,yy,col=4)
#Box kernel
lines(c(-2,-1,-1,1,1,2),c(0,0,1/2,1/2,0,0),col=5)
#Triangular kernel
lines(c(-2,-1,0,1,2),c(0,0,1,0,0),col=6)
legend("topleft", legend=c("tri-cube", "Epanechnikov", "Gaussian", "Box", "Triangl
e''), lty=1, col=c(1,3,4,5,6))
```



Example: Scatterplot smoothers (Loess)

In this example, we are going to work with the diabetes data set from the start of this section. This is data from a study of the factors affecting patterns of insulin-dependent diabetes mellitus in children, Sockett et al. 1987.

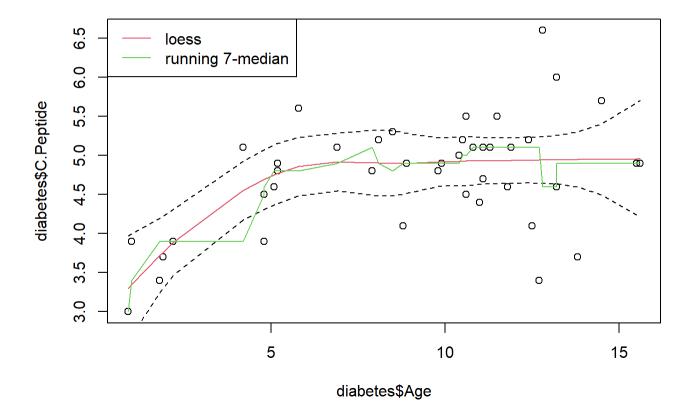
diabetes <- read.table("diabetes.dat", header=TRUE, quote="\"")
diabetes <- diabetes[order(diabetes\$Age),] #put the age in ascending order (not neces
sary here)
head(diabetes)</pre>

	Age <dbl></dbl>	Base.Deficit <dbl></dbl>	C.Peptide <dbl></dbl>
15	0.9	-11.6	3.0
24	1.0	-8.2	3.9
6	1.8	-19.2	3.4
10	1.9	-25.0	3.7
11	2.2	-3.1	3.9
36	4.2	-17.0	5.1

The scatterplot smoothers for the diabetes data set were obtained as follows:

```
plot(diabetes$Age, diabetes$C.Peptide, main="Diabetes Data")
# loess: Fit a polynomial surface determined by one or more numerical predictors, usi
ng local fitting.
#The size of the neighborhood can be controlled using the span argument, which ranges
between 0 to 1. It controls the degree of smoothing. So, the greater the value of spa
n, more smooth is the fitted curve. Default span=0.75
fit=loess(diabetes$C.Peptide~diabetes$Age,diabetes)
# predict: Predictions from a loess fit, optionally with standard errors,
# se: should standard errors be computed?
pred=predict(fit,diabetes$Age,se=T)
# df in the output stands for effective degrees of freedom (Page 278-279 ISLR)
lines(diabetes$Age,predict(fit),col=2)
# Confidence interval
lines(diabetes$Age,pred$fit+2*pred$se.fit,lty=2)
lines(diabetes$Age,pred$fit-2*pred$se.fit,lty=2)
# runmed: Compute running medians of odd span
lines(diabetesAge,runmed(x = diabetes\\C.Peptide,k = 7),col=3)
legend("topleft", legend = c("loess", "running 7-median"), lty=<math>c(1,1), col = 2:3)
```

Diabetes Data



```
# lines(loess.smooth(diabetes$Age, diabetes$C.Peptide, span=0.75),col=6)
# The function loess.smooth: returns a list with two components, x and y. x contains
a set of predictor values and y is the vector of smoothed values given by loess.smoot
h. The default specification of k in loess.smooth is a "span" of 2/3 of all data valu
es.
#lines(loess.smooth(diabetes$Age, diabetes$C.Peptide),col=2)
```

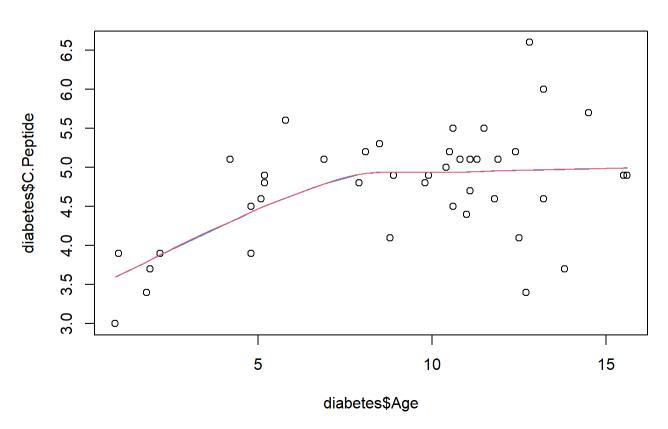
If you set the parameters of loess. smooth function and loess function the same, you will end up with smooth carves very close to each other. Please run the following code:

```
plot(diabetes$Age,diabetes$C.Peptide,main="Diabetes Data")

fit=loess(C.Peptide~Age,data= diabetes, span = 0.75,family = "symmetric", degree=1)
# in loess function the degree of the polynomials are normally 1 or 2.
pred=predict(fit,diabetes$Age,se=T)
lines(diabetes$Age,predict(fit),col=4)

fit1=loess.smooth(diabetes$Age, diabetes$C.Peptide, span = 0.75,family = "symmetric", degree=1)
lines(fit1,col=2)
```

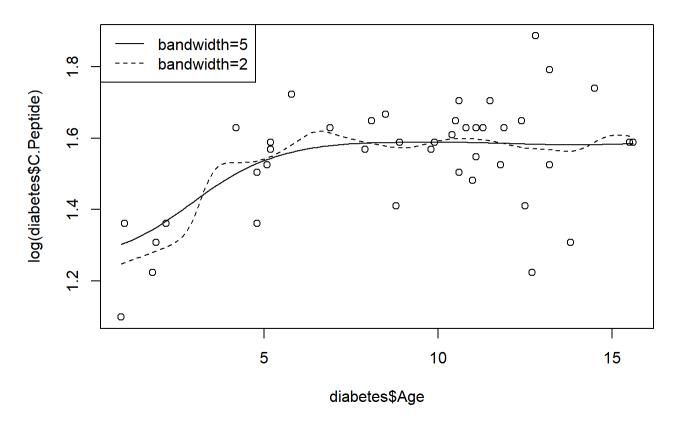
Diabetes Data



Example: Kernel smoothing

In this example we illustrate kernel smoothing for the diabetes data (with log(C. peptide) as the response and age as the predictor):

Kernel smooth



As for loess.smooth(), the output of the function ksmooth() is a list with components x and y (numeric vectors, by default x is the set of observed predictors and y gives corresponding values of the kernel smooth).

The argument bandwidth controls the degree of smoothing (the default value is usually not sensible) and kernel allows specification of the kernel (options box and normal, see help for details).

Example: Local likelihood

Recall the trade union data set, which we have used as an example for logistic regression. The package locfit fits a nonparametric logistic regression model as follows:

```
library(SemiPar)

data("trade.union")
attach(trade.union)
require(locfit)
```

locfit 1.5-9.8

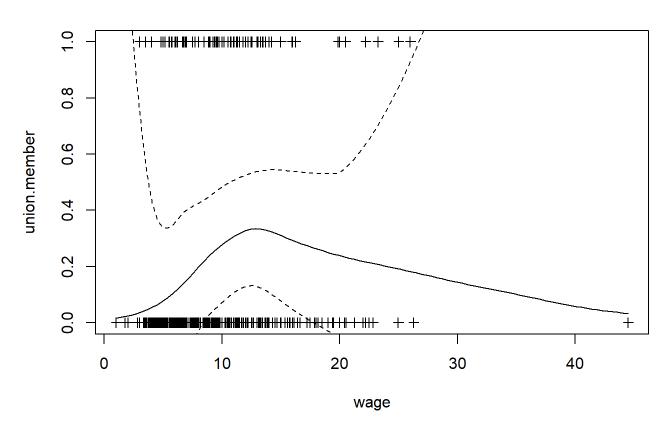
Loading required package: locfit

2023-06-11

```
#locfit: is the model formula-based interface for fitting local regression and likeli
hood models.
# lp: is a local polynomial model term for Locfit models. Usually, it will be the onl
y term on the RHS of the model formula.
  #nn: Nearest neighbor component of the smoothing parameter. Default value is 0.7, u
nless either h or adpen are provided, in which case the default is 0.
        : The constant component of the smoothing parameter. Default: 0.
fit=locfit(union.member~lp(wage,nn=0.7,deg=2), data=trade.union,family="binomial")
plot(fit,ylim = c(0,1),type='n',main="Trade Union Data")
newxx=seq(from = min(wage), to = max(wage), length.out = 100)
newdat=data.frame(wage=newxx)
ypred=predict(fit,newdat,se.fit = T)
lines(newxx,ypred$fit)
lines(newxx,ypred$fit-ypred$se.fit,lty=2)
lines(newxx,ypred$fit+ypred$se.fit,lty=2)
# jitter: Add a small amount of noise to a numeric vector
```

points(jitter(wage), union.member, main = "trade union data set", pch = 3)

Trade Union Data



Activity in R 1: Loess Smoother

Download the data set ethanol. The ethanol data frame contains 88 measurements generated in an experiment in which ethanol was burned in a single cylinder automobile test engine. The variables are NOx (a measure of the nitrogen oxides in the exhaust), C (compression ratio of an engine) and E (a measure of the richness of the air/ethanol mix used).

```
ethanol<-read.table("ethanol.txt",header=T)
# data in SemiPar package
print(dim(ethanol))</pre>
```

[1] 88 3

head(ethanol)

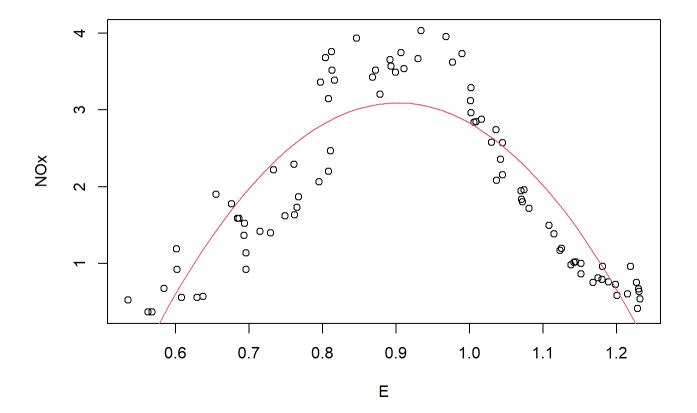
	NOx <dbl></dbl>	C <dbl></dbl>	E <dbl></dbl>
1	3.741	12	0.907
2	2.295	12	0.761
3	1.498	12	1.108

	NOx <dbl></dbl>	C <dbl></dbl>	E <dbl></dbl>
4	2.881	12	1.016
5	0.760	12	1.189
6	3.120	9	1.001
6 rows			

attach(ethanol)

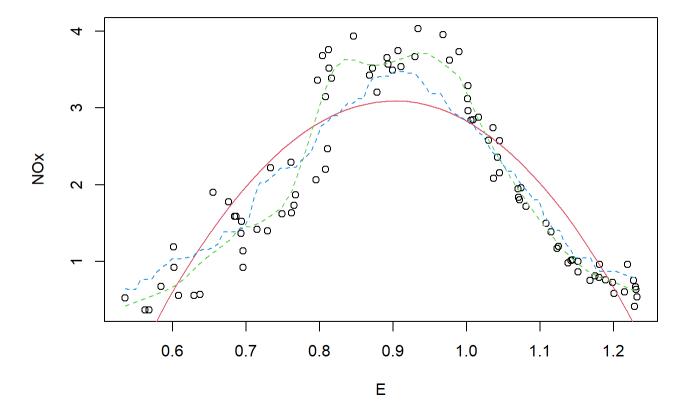
a. Do a scatterplot of NOx against E. After looking at the scatterplot you might suggest a polynomial regression model to capture the relationship between the response NOx and the predictor E. Fit a quadratic regression model and superimpose the fitted curve on the scatterplot.

```
plot(E, N0x)
Esq<-E*E
ethanol.lm<-lm(N0x~E+Esq)
Egrid<-seq(from=min(E),to=max(E),length=50)
new.data<-data.frame(E=Egrid,Esq=Egrid*Egrid)
ethanol.pred<-predict(ethanol.lm,newdata=new.data)
lines(Egrid,ethanol.pred,col=2)</pre>
```



b. Superimpose on the scatterplot in a) a suitable loess smooth. Do you think the smooth captures structure in the data that is missed by the quadratic regression model?

```
plot(E, NOx)
Esq<-E*E
ethanol.lm<-lm(NOx~E+Esq)
Egrid<-seq(from=min(E),to=max(E),length=50)
new.data<-data.frame(E=Egrid,Esq=Egrid*Egrid)
ethanol.pred<-predict(ethanol.lm,newdata=new.data)
lines(Egrid,ethanol.pred,col=2)
lines(loess.smooth(E,NOx,span=0.2),lty=2,col=3)
lines(ksmooth(E,NOx,bandwidth=0.2),lty=2,col=4)</pre>
```



From the above figure, it seems that loess smooth capture more bell-shaped structure of the data. This is slightly different from the quadratic regression fit.

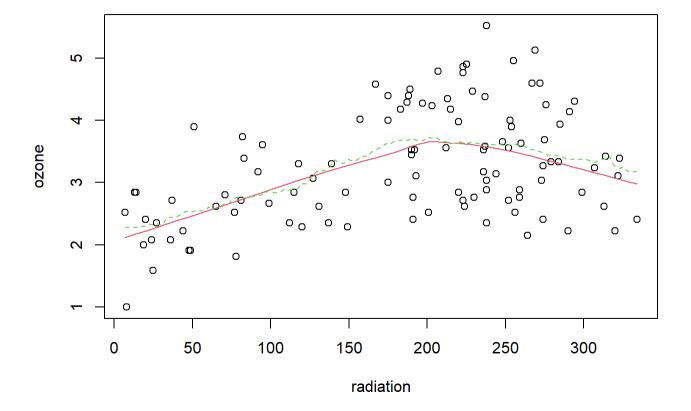
```
# library(fANCOVA)
# degree: the degree of the local polynomials to be used. It can ben 0, 1 or 2
# Fit a local polynomial regression with automatic smoothing parameter selection.
# fit_loess <- loess.as(E,NOx, degree = 1, criterion = "gcv", user.span = NULL, plot
= T)
# summary(fit_loess)</pre>
```

Activity in R: Kernel Smoother

Download the data set air (there are four columns in this data frame, ozone, radiation, temperature and wind). The data set records New York Air Quality Measurements, May to September 1973.

Plot a scatterplot of ozone against radiation and superimpose loess and kernel smooths on the scatterplot. You may need to change the default level of smoothing for the kernel and loess smooths.

```
air<-read.table("air.txt",header=T)
attach(air)
plot(radiation,ozone)
# loess.smooth:Plot and add a smooth curve computed by loess to a scatter plot. You c
an add degree as a parameter # default span=2/3
lines(loess.smooth(radiation,ozone),col=2)
lines(ksmooth(radiation,ozone,bandwidth=100),lty=2,col=3)</pre>
```



bandwidth: the bandwidth. The kernels are scaled so that their quartiles (viewed as probability densities) are at \pm 0.25*bandwidth.

Section 5.2 Polynomial regression and step functions

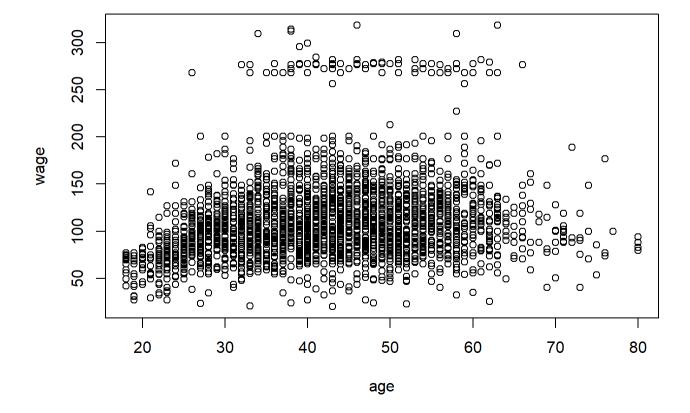
Example: Polynomial regression

In this example we analyze the Wage data from the ISLR library.

```
library(ISLR)
data("Wage")
attach(Wage)

## The following objects are masked from trade.union:
##
## age, race, wage

plot(age,wage)
```



```
fit=lm(wage~poly(age,4,raw=T), data=Wage)
# if true, use raw and not orthogonal polynomials
coef(summary(fit))
```

```
## (Intercept) -1.841542e+02 6.004038e+01 -3.067172 0.0021802539

## poly(age, 4, raw = T)1 2.124552e+01 5.886748e+00 3.609042 0.0003123618

## poly(age, 4, raw = T)2 -5.638593e-01 2.061083e-01 -2.735743 0.0062606446

## poly(age, 4, raw = T)3 6.810688e-03 3.065931e-03 2.221409 0.0263977518

## poly(age, 4, raw = T)4 -3.203830e-05 1.641359e-05 -1.951938 0.0510386498
```

There are several other equivalent ways of fitting this model:

```
fit2=lm(wage~age+I(age^2)+I(age^3)+I(age^4),data=Wage)
coef(summary(fit2))
```

```
## https://stackoverflow.com/questions/24192428/what-does-the-capital-letter-i-in-r-l
inear-regression-formula-mean
## https://stackoverflow.com/questions/8055508/in-r-formulas-why-do-i-have-to-use-th
e-i-function-on-power-terms-like-y-i
```

or

```
fit3=lm(wage~cbind(age,age^2,age^3,age^4),data=Wage)
coef(summary(fit3))
```

```
##
                                          Estimate
                                                     Std. Error
                                                                t value
                                     -1.841542e+02 6.004038e+01 -3.067172
## (Intercept)
## cbind(age, age^2, age^3, age^4)age 2.124552e+01 5.886748e+00 3.609042
## cbind(age, age^2, age^3, age^4)
                                     -5.638593e-01 2.061083e-01 -2.735743
## cbind(age, age^2, age^3, age^4) 6.810688e-03 3.065931e-03 2.221409
## cbind(age, age^2, age^3, age^4)
                                     -3.203830e-05 1.641359e-05 -1.951938
##
                                         Pr(>|t|)
## (Intercept)
                                     0.0021802539
## cbind(age, age^2, age^3, age^4)age 0.0003123618
## cbind(age, age^2, age^3, age^4)
                                     0.0062606446
## cbind(age, age^2, age^3, age^4)
                                     0.0263977518
## cbind(age, age^2, age^3, age^4)
                                     0.0510386498
```

Note the difference to the following code:

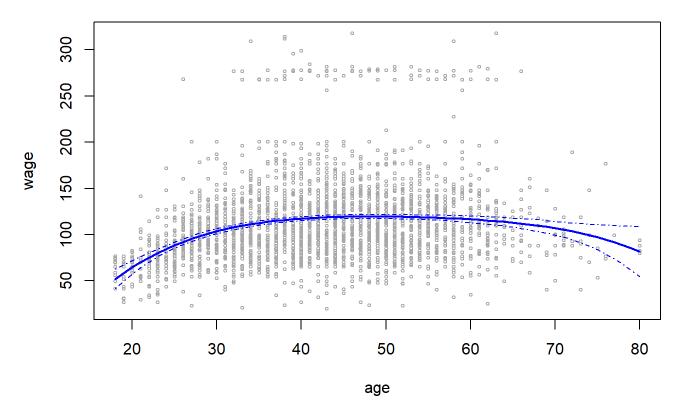
```
fit4=lm(wage~age+age^2+age^3+age^4,data=Wage)
coef(summary(fit4))
```

```
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 81.7047354 2.84624224 28.70618 2.543375e-160
## age 0.7072759 0.06475113 10.92299 2.900778e-27
```

Let us now fit the degree-4 polynomial to wage as a function of age in the Wage dataset.

```
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.fit, preds$fit-2*preds$se.fit)
par(mfrow=c(1,1),mar=c(4.5,4.5,1,1),oma=c(0,0,4,0))
plot(age,wage,xlim=agelims, cex=.5,col="darkgrey")
title("Degree-4 Polynomial", outer=T)
lines(age.grid, preds$fit, lwd=2, col="blue")
# matlines Plot the columns of one matrix against the columns of another
matlines(age.grid, se.bands, lwd=1,col="blue",lty=4)
```

Degree-4 Polynomial



Below we also illustrate one way of choosing the degree of the polynomial to use. We now fit models ranging from linear to a degree-5 polynomial and use hypothesis tests to determine the simplest model which is sufficient to explain the relationship between wage and age.

```
fit.1=lm(wage~age,data=Wage)
fit.2=lm(wage~poly(age,2),data=Wage)
fit.3=lm(wage~poly(age,3),data=Wage)
fit.4=lm(wage~poly(age,4),data=Wage)
fit.5=lm(wage~poly(age,5),data=Wage)
anova(fit.1,fit.2,fit.3,fit.4,fit.5)
```

	Res.Df <dbl></dbl>	RSS <dbl></dbl>	Df <dbl></dbl>	Sum of Sq <dbl></dbl>	F <dbl></dbl>	Pr(>F) <dbl></dbl>
1	2998	5022216	NA	NA	NA	NA
2	2997	4793430	1	228786.010	143.5931074	2.367734e-32
3	2996	4777674	1	15755.694	9.8887559	1.679213e-03
4	2995	4771604	1	6070.152	3.8098134	5.104623e-02
5	2994	4770322	1	1282.563	0.8049758	3.696820e-01
5 row	/S					

The p-value corresponding to comparing linear Model1 to the quadratic Model2 is small indicating that a linear fit is not sufficient. The p-value corresponding to comparing Model2 to Model3 is also low indicating that Model2 is not sufficient. The p-value corresponding to comparing Model3 and Model4 is greater than 0.05 indicating that there is no sufficient improvement in choosing degree-4 polynomial over the cubic polynomial. Hence the cubic polynomial appears to provide a reasonable fit to the data.

Note that as an alternative to using ANOVA, we could choose the polynomial degree using cross-validation.

Example: polynomial logistic regression

We consider a procedure for predicting whether an individual earns more than \$250,000 per year.

```
fit=glm(I(wage>250)~poly(age,4),data=Wage,family=binomial)

agelims=range(age)
age.grid=seq(from=agelims[1], to=agelims[2])

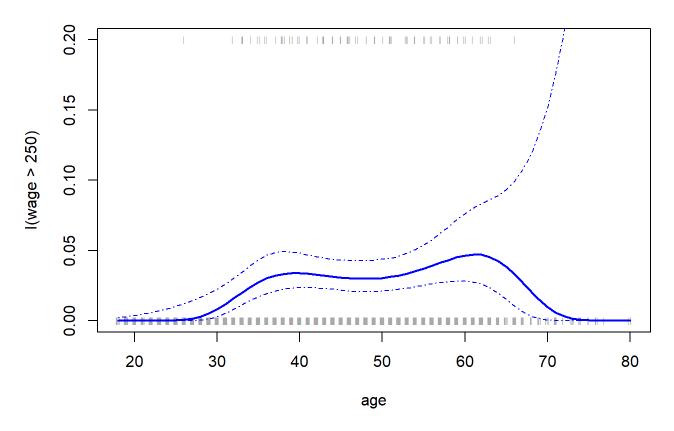
preds=predict(fit, newdata=list(age=age.grid),se=T)
pfit=exp(preds$fit)/(1+exp(preds$fit))
se.bands.logit=cbind(preds$fit+2*preds$se.fit,preds$fit-2*preds$se.fit)
se.bands=exp(se.bands.logit)/(1+exp(se.bands.logit))
```

In order to directly compute the probabilities we select type =" response " in predict() as follows:

```
preds=predict(fit,newdata=list(age=age.grid),type="response",se=T)
```

For visualization we execute the following code:

```
plot(age, I(wage>250),xlim=agelims, type="n", ylim=c(0,0.2))
points(jitter(age), I((wage>250)/5), cex=.5,pch="|",col="darkgrey")
lines(age.grid,pfit, lwd=2, col="blue")
matlines(age.grid, se.bands, lwd=1, col="blue", lty=4)
```



Note the wide confidence intervals on the right-hand side. Although the sample size for this data is large (3,000), there are only 79 high earners, which results in high variance in the estimated coefficients.

```
fit.1=glm(I(wage>250)~poly(age,1),data=Wage,family=binomial)
fit.2=glm(I(wage>250)~poly(age,2),data=Wage,family=binomial)
fit.3=glm(I(wage>250)~poly(age,3),data=Wage,family=binomial)
fit.4=glm(I(wage>250)~poly(age,4),data=Wage,family=binomial)
fit.5=glm(I(wage>250)~poly(age,5),data=Wage,family=binomial)
```

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

```
#AIC=c(fit.1$aic,fit.2$aic,fit.3$aic,fit.4$aic,fit.5$aic )
anova(fit.1,fit.2,fit.3,fit.4,fit.5, test="Chisq")
```

	Resid. Df <dbl></dbl>	Resid. Dev <dbl></dbl>	Df <dbl></dbl>	Deviance <dbl></dbl>	Pr(>Chi) <dbl></dbl>
1	2998	719.2285	NA	NA	NA
2	2997	709.0237	1	10.204766	0.001400782
3	2996	707.9215	1	1.102191	0.293785708
4	2995	701.2198	1	6.701683	0.009632195

	Resid. Df <dbl></dbl>	Resid. Dev <dbl></dbl>	Df <dbl></dbl>	Deviance <dbl></dbl>	Pr(>Chi) <dbl></dbl>
5	2994	698.8699	1	2.349930	0.125288656
5 rows					

```
anova(fit.1,fit.2,fit.4,fit.5, test="Chisq")
```

	Resid. Df <dbl></dbl>	Resid. Dev <dbl></dbl>	Df <dbl></dbl>	Deviance <dbl></dbl>	Pr(>Chi) <dbl></dbl>
1	2998	719.2285	NA	NA	NA
2	2997	709.0237	1	10.204766	0.001400782
3	2995	701.2198	2	7.803874	0.020202739
4	2994	698.8699	1	2.349930	0.125288656
4 rows					

https://stackoverflow.com/questions/67360883/how-to-fix-fitted-probabilities-numer
ically-0-or-1-occurred-warning-in-r

Example: step functions

This example illustrates how to fit a step function in R using cut():

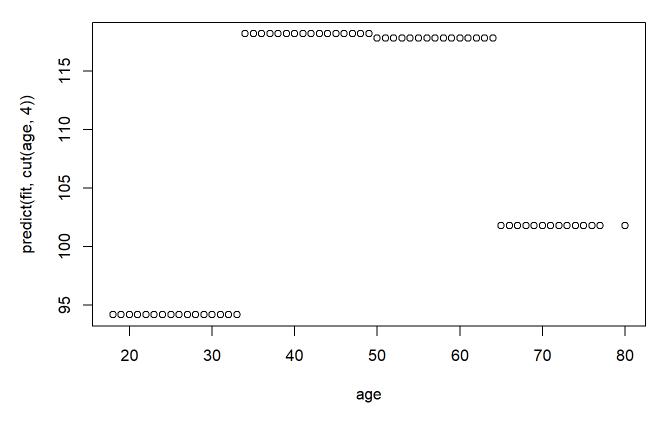
```
\# cut: cut divides the range of x into intervals and codes the values in x according to which interval they fall. table(cut(age,breaks=4))
```

```
##
## (17.9,33.5] (33.5,49] (49,64.5] (64.5,80.1]
## 750 1399 779 72
```

```
fit=lm(wage~cut(age,4),data=Wage)
coef(summary(fit))
```

```
## (Intercept) 94.158392 1.476069 63.789970 0.0000000e+00
## cut(age, 4)(33.5,49] 24.053491 1.829431 13.148074 1.982315e-38
## cut(age, 4)(49,64.5] 23.664559 2.067958 11.443444 1.040750e-29
## cut(age, 4)(64.5,80.1] 7.640592 4.987424 1.531972 1.256350e-01
```

```
plot(age,predict(fit,cut(age,4)))
```



Note that the cut() function returns an ordered categorical variable and lm() function creates a set of dummy variables for use in the regression.

Activity in R: Polynomial regression

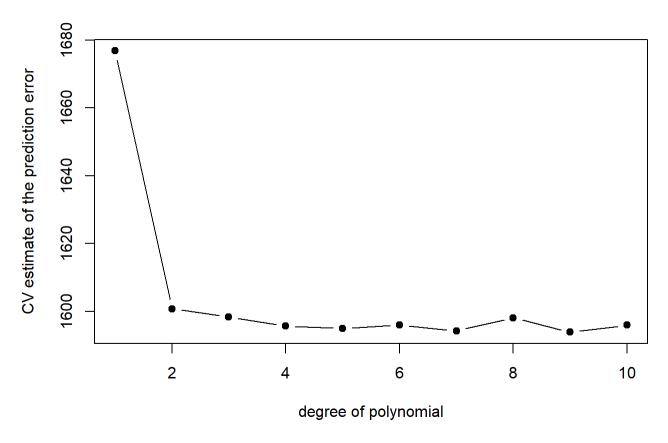
In this activity, you will further analyse the Wage data set considered in this section. Perform polynomial regression to predict wage using age. Use cross-validation to select the optimal degree d for the polynomial. What degree was chosen, and how does this compare to the results of hypothesis testing using ANOVA? Make a plot of the resulting polynomial fit to the data.

First we will perform polynomial regression for various polynomial degrees

```
library(boot) # Bootstrap Functions
set.seed(1)
cv.error = rep(0,10)
for( i in 1:10 ){
   glm.fit = glm( wage ~ poly(age,i), data=Wage )
   # cv.glm: This function calculates the estimated K-fold cross-validation prediction
error for generalized linear models.
   cv.error[i] = cv.glm( Wage, glm.fit, K=10 )$delta[1]
}
#delta[1]: raw cross-validation estimate of prediction error
#delta[2]: the adjusted cross-validation estimate of prediction error
```

And plot the cross-validation errors:

```
plot( 1:10, cv.error, pch=19, type='b', xlab='degree of polynomial', ylab='CV estimat e of the prediction error' )
```



The minimal CV-error corresponds to the degree of the polynomial equal to

```
me = which.min( cv.error )
me
```

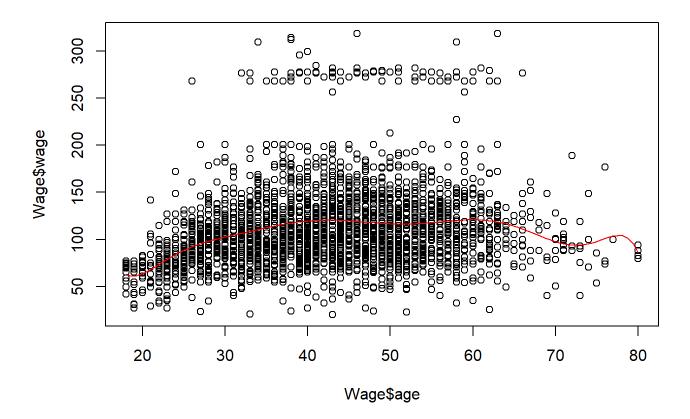
```
## [1] 9
```

Hence:

```
m = glm( wage ~ poly(age,me), data=Wage )
```

The polynomial fit plot can be obtained as follows:

```
plot( Wage$age, Wage$wage )
aRng = range(Wage$age)
a_predict = seq( from=aRng[1], to=aRng[2], length.out=100 )
w_predict = predict( m, newdata=list( age=a_predict ) )
lines( a_predict, w_predict, col='red' )
```



Section 5.3 Regression splines

{} To fit a spline we need to select the order of the spline, the number of knots and their placement.

bs(x, df = 7) in R generates a basis matrix of cubic spline functions evaluated at the N observations in x, with the 7 - 3 = 4 interior knots at the respective percentiles of x.

bs(x, degree = 1, knots = c(0.2, 0.4, 0.6)) generates a basis for linear splines, with the three interior knots.

Warning: by default the bs() function does not take the intercept into account. Therefore df = length(knots) + degree. The intercept can be included by specifying bs(..., intercept=TRUE).

Example: A linear spline with two knots (red) and 50 knots (green):

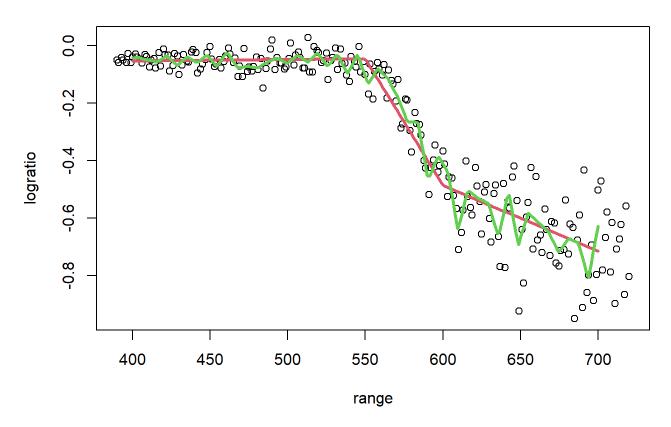
```
library(SemiPar)
require(splines) #Regression Spline Functions and Classes
```

Loading required package: splines

```
## Loading required package: splines
data(lidar)
attach(lidar)
range(lidar$range)
## [1] 390 720
# bs: Generate the B-spline basis matrix for a polynomial spline. The default value f
or degree is 3.
fit <- lm(logratio \sim bs(x = range, knots = c(550,600), degree = 1))
attr(terms(fit), "predvars")
## list(logratio, bs(x = range, degree = 1L, knots = c(550, 600),
       Boundary.knots = c(390L, 720L), intercept = FALSE))
##
fit2<- lm(logratio \sim bs(x = range, df = 51, degree = 1))
attr(terms(fit2), "predvars")
## list(logratio, bs(x = range, degree = 1L, knots = c(396.313725490196,
## 402.627450980392, 408.941176470588, 415.509803921569, 422.137254901961,
## 428.764705882353, 435.196078431373, 441.509803921569, 447.823529411765,
## 454.274509803922, 460.901960784314, 467.529411764706, 474.078431372549,
## 480.392156862745, 486.705882352941, 493.039215686275, 499.666666666667,
## 506.294117647059, 512.921568627451, 519.274509803922, 525.588235294118,
## 531.901960784314, 538.43137254902, 545.058823529412, 551.686274509804,
## 558.156862745098, 564.470588235294, 570.78431372549, 577.196078431372,
## 583.823529411765, 590.450980392157, 597.039215686274, 603.352941176471,
## 609.66666666667, 615.980392156863, 622.588235294118, 629.21568627451,
## 635.843137254902, 642.235294117647, 648.549019607843, 654.862745098039,
## 661.352941176471, 667.980392156863, 674.607843137255, 681.117647058824,
## 687.43137254902, 693.745098039216, 700.117647058824, 706.745098039216,
## 713.372549019608), Boundary.knots = c(390L, 720L), intercept = FALSE))
```

```
plot(lidar, main = "LIDAR data")
xpred <- seq(400,700, length.out = 200)
lines(xpred, predict(fit, data.frame(range = xpred)),col=2,lwd=3)
lines(xpred, predict(fit2, data.frame(range = xpred)),col=3,lwd=3)</pre>
```

LIDAR data



For the LIDAR data set, the basis 1, x, (x-550)+, (x-600)+ was chosen, where we have defined $x_+ = \max\{x, 0\}$. The design matrix is

$$X = \begin{bmatrix} 1 & x_1 & (x_1 - 550)_+ & (x_1 - 600)_+ \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & (x_n - 550)_+ & (x_n - 600)_+ \end{bmatrix}.$$

Here 550 and 600 are called knots, and $(x_1 - 500)_+$ are linear spline functions. Linear combinations of linear spline functions are all piecewise linear.

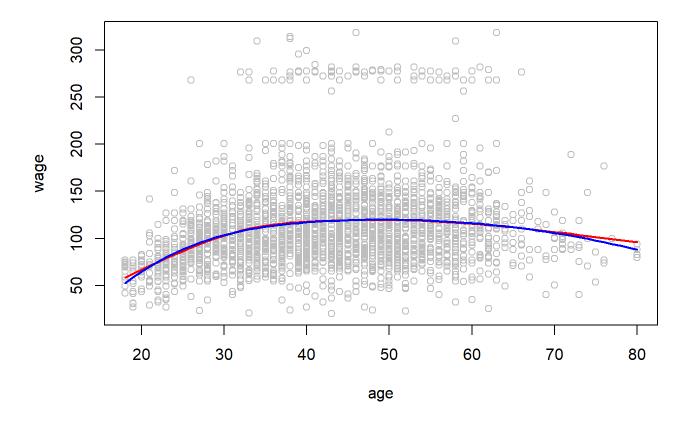
```
# fit3 <- lm(logratio \sim ns(x = range, knots = c(550,600)))
# fit4<- lm(logratio \sim ns(x = range, df = 11))
# plot(lidar, main = "LIDAR data")
# xpred <- seq(400,700, length.out = 200)
# lines(xpred, predict(fit3, data.frame(range = xpred)), col=2, lwd=3)
# lines(xpred, predict(fit4, data.frame(range = xpred)), col=3, lty=2, lwd=3)
```

Example: natural spline (red) and ordinary spline (blue)

In order to fit a natural spline, we use the ns() function as follows:

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

```
## The following objects are masked from Wage (pos = 6):
##
       age, education, health, health ins, jobclass, logwage, maritl,
##
       race, region, wage, year
##
## The following objects are masked from trade.union:
##
##
       age, race, wage
library(splines)
agelims=range(age)
age.grid=seq(from=agelims[1], to=agelims[2])
# ns: Generate the B-spline basis matrix for a natural cubic spline
# https://stats.stackexchange.com/questions/360993/number-of-basis-functions-in-natur
al-cubic-spline
fit=lm(wage~ns(age, df=4),data=Wage)
## To see what knots were selected
attr(terms(fit), "predvars") # attr in base library
## list(wage, ns(age, knots = c(33.75, 42, 51), Boundary.knots = c(18L, 42, 51)
## 80L), intercept = FALSE))
# In ns(), df - 1 - intercept=knots ---> 4-1-0=3
fit2=lm(wage~bs(age,df=4), data=Wage)
attr(terms(fit2), "predvars")
## list(wage, bs(age, degree = 3L, knots = 42, Boundary.knots = c(18L,
## 80L), intercept = FALSE))
#In bs, df - degree - intercept=knots ---> 4-3-0=1
# Boundry.knots: max and min
pred=predict(fit,newdata=list(age=age.grid),se=T)
pred2=predict(fit2,newdata=list(age=age.grid),se=T)
plot(age, wage, col="grey")
lines(age.grid,pred$fit,col="red",lwd=2)
lines(age.grid,pred2$fit,col="blue", lwd=2)
```



Other examples in https://datascienceplus.com/cubic-and-smoothing-splines-in-r/

Activity: Spline Regression

This question uses the variables dis (the weighted mean of distances to five Boston employment centers) and nox (nitrogen oxides concentration in parts per 10 million) from the Boston data. We will treat dis as the predictor and nox as the response.

Part 1

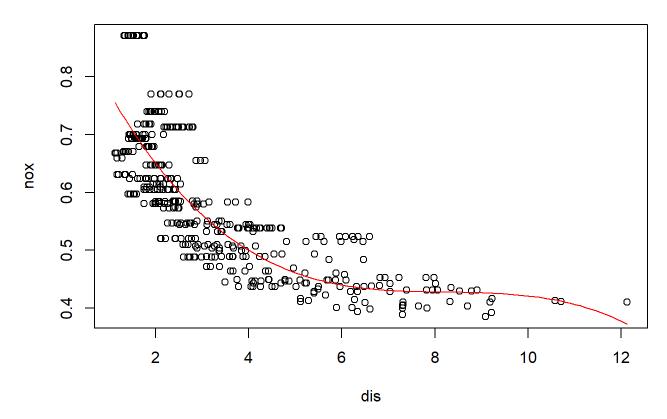
Use the poly() function to fit a cubic polynomial regression to predict nox using dis. Report the regression output, and plot the resulting data and polynomial fits. Note that for this question and the following, we will consider an orthogonal polynomial basis, leaving the default argument raw = FALSE.

```
library(MASS)
m = lm( nox ~ poly(dis,3), data=Boston )
summary(m)
```

```
##
## Call:
## lm(formula = nox ~ poly(dis, 3), data = Boston)
##
## Residuals:
##
        Min
                   1Q
                         Median
                                       30
                                                Max
## -0.121130 -0.040619 -0.009738 0.023385
                                          0.194904
##
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                 0.554695
                            0.002759 201.021 < 2e-16 ***
                            0.062071 -32.271 < 2e-16 ***
## poly(dis, 3)1 -2.003096
## poly(dis, 3)2 0.856330
                            0.062071 13.796 < 2e-16 ***
## poly(dis, 3)3 -0.318049
                            0.062071 -5.124 4.27e-07 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.06207 on 502 degrees of freedom
## Multiple R-squared: 0.7148, Adjusted R-squared: 0.7131
## F-statistic: 419.3 on 3 and 502 DF, p-value: < 2.2e-16
```

```
plot( Boston$dis, Boston$nox, xlab='dis', ylab='nox', main='third degree polynomial f
it' )
dis_range = range( Boston$dis )
dis_samples = seq( from=dis_range[1], to=dis_range[2], length.out=100 )
y_hat = predict( m, newdata=list( dis=dis_samples ) )
lines( dis_samples, y_hat, col='red' )
```

third degree polynomial fit



The data is fit quite well with this third order polynomial as the plot and the R output shows.

Part 2

Plot the polynomial fits for a range of different polynomial degrees (say, from 1 to 10), and report the associated residual sum of squares.

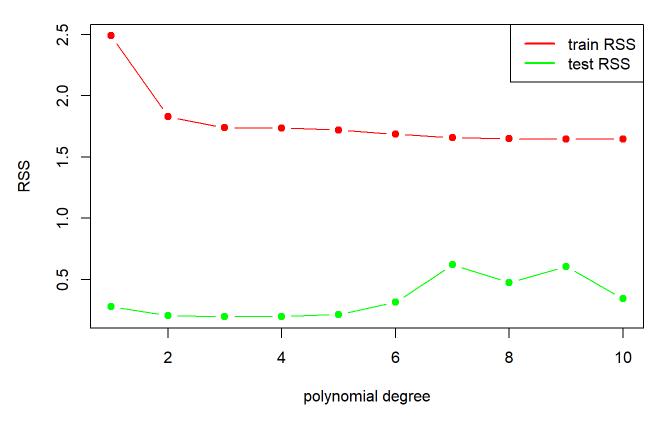
```
d_max = 10
# The training RSS:
training_rss = rep(NA,d_max)
for( d in 1:d_max ){
    m = lm( nox ~ poly(dis,d), data=Boston )
    training_rss[d] = sum( ( m$residuals )^2 )
}
training_rss
```

```
## [1] 2.768563 2.035262 1.934107 1.932981 1.915290 1.878257 1.849484 1.835630
## [9] 1.833331 1.832171
```

Part 3

Perform cross-validation or another approach to select the optimal degree for the polynomial, and explain your results.

```
set.seed(1)
k = 10
d \max = 10
folds = sample( 1:k, nrow(Boston), replace=TRUE )
#takes a sample from 1:k and with replacement (value 1 to k repeated sevaral times)
cv.rss.test = matrix( NA, k, d max )
cv.rss.train = matrix( NA, k, d max )
for( d in 1:d max ){
  for( fi in 1:k ){ # for each fold
    fit = lm( nox ~ poly(dis,d), data=Boston[folds!=fi,] )
    y hat = predict( fit, newdata=Boston[folds!=fi,] )
    cv.rss.train[fi,d] = sum( ( Boston[folds!=fi,]$nox - y hat )^2 )
    y hat = predict( fit, newdata=Boston[folds==fi,] )
    cv.rss.test[fi,d] = sum( ( Boston[folds==fi,]$nox - y hat )^2 )
 }
}
cv.rss.train.mean = apply(cv.rss.train,2,mean)
cv.rss.train.stderr = apply(cv.rss.train,2,sd)/sqrt(k)
cv.rss.test.mean = apply(cv.rss.test,2,mean)
cv.rss.test.stderr = apply(cv.rss.test,2,sd)/sqrt(k)
min value = min( c(cv.rss.test.mean,cv.rss.train.mean) )
max value = max( c(cv.rss.test.mean,cv.rss.train.mean) )
plot( 1:d max, cv.rss.train.mean, xlab='polynomial degree', ylab='RSS', col='red', pc
h=19, type='b', ylim=c(min value,max value) )
lines( 1:d max, cv.rss.test.mean, col='green', pch=19, type='b' )
legend( "topright", legend=c("train RSS","test RSS"), col=c("red","green"), lty=1, lw
d=2
```



The training RSS steadily decreases as we add more degrees of freedom. The testing RSS decreases initially (to a low at a degree of around three) and then begins to increase again as the degree of the polynomial gets larger. Form this plot a degree three polynomial seems to be optimal.

Part 4

Use the bs() function to fit a regression spline to predict nox using dis. How would you choose the knots? Plot the resulting fit. Report the output for the fit using four degrees of freedom.

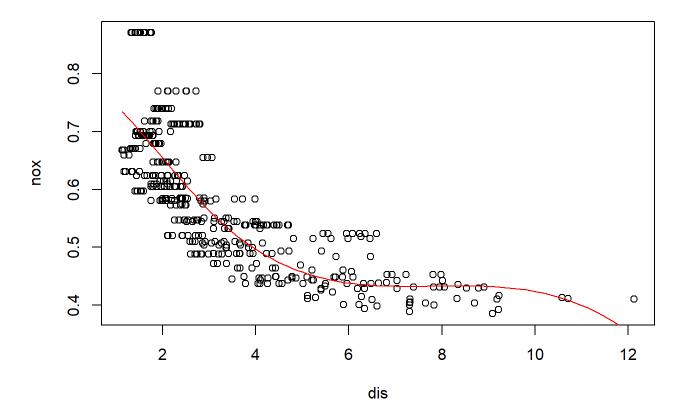
```
library(MASS)
library(splines)
m = lm( nox ~ bs(dis,df=4), data=Boston ) # defualt degree=3
plot( Boston$dis, Boston$nox, xlab='dis', ylab='nox', main='bs with df=4 fit' )
attr(terms(m), "predvars")

## list(nox, bs(dis, degree = 3L, knots = 3.20745, Boundary.knots = c(1.1296,
## 12.1265), intercept = FALSE))

# knots=median(Boston$dis)

dis_range = range( Boston$dis )
dis_samples = seq( from=dis_range[1], to=dis_range[2], length.out=100 )
y_hat = predict( m, newdata=list( dis=dis_samples ) )
lines( dis samples, y hat, col='red' )
```

bs with df=4 fit



Part 5

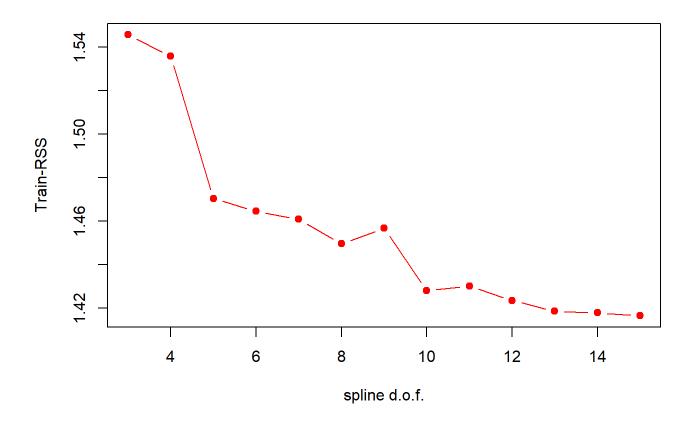
Now fit a regression spline for a range of degrees of freedom, and plot the resulting fits and report the resulting RSS. Describe the results obtained.

Next, perform cross-validation or another approach to select the best degrees of freedom for a regression spline on this data. Describe your results.

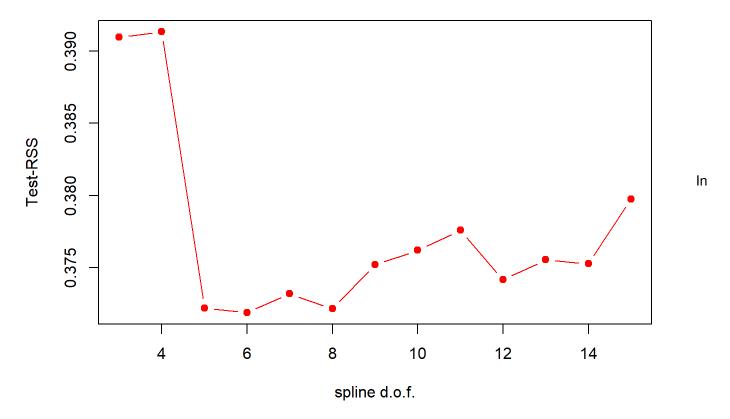
```
set.seed(1)
dof choices = c(3:15)
n dof choices = length(dof choices)
# The RSS estimated using cross-validation:
k = 5
folds = sample( 1:k, nrow(Boston), replace=TRUE )
cv.rss.test = matrix( NA, k, n dof choices )
cv.rss.train = matrix( NA, k, n dof choices )
for( di in 1:n dof choices ){
  for( fi in 1:k ){ # for each fold
    fit = lm( nox ~ bs(dis,df=dof choices[di]), data=Boston[folds!=fi,] )
    y hat = predict( fit, newdata=Boston[folds!=fi,] )
    cv.rss.train[fi,di] = sum( ( Boston[folds!=fi,]$nox - y hat )^2 )
    y hat = predict( fit, newdata=Boston[folds==fi,] )
    cv.rss.test[fi,di] = sum( ( Boston[folds==fi,]$nox - y hat )^2 )
 }
}
## Warning in bs(dis, degree = 3L, knots = numeric(0), Boundary.knots = c(1.137, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = 3.2721, Boundary.knots = c(1.137, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(2.39623333333333, 4.37753333333333:
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(2.1103, 3.2721, 5.25095),
## Boundary.knots = c(1.137, : some 'x' values beyond boundary knots may cause
## ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.9784, 2.7006, 3.8473, 5.885), :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.8755, 2.39623333333333, 3.2721, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.8008, 2.2271, 2.78198571428571, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
```

```
## Warning in bs(dis, degree = 3L, knots = c(1.750125, 2.1103, 2.516825, 3.2721, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.66397777777778, 2.046655555555556, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.6232, 1.9784, 2.2875, 2.7006, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.60862727272727, 1.92090909090909, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.58941666666667, 1.8755, 2.1103, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
## Warning in bs(dis, degree = 3L, knots = c(1.57749230769231, 1.82353076923077, :
## some 'x' values beyond boundary knots may cause ill-conditioned bases
cv.rss.train.mean = apply(cv.rss.train,2,mean)
cv.rss.train.stderr = apply(cv.rss.train,2,sd)/sqrt(k)
cv.rss.test.mean = apply(cv.rss.test,2,mean)
cv.rss.test.stderr = apply(cv.rss.test,2,sd)/sqrt(k)
min value = min( c(cv.rss.test.mean,cv.rss.train.mean) )
max value = max( c(cv.rss.test.mean,cv.rss.train.mean) )
plot( dof_choices, cv.rss.train.mean, xlab='spline d.o.f.', ylab='Train-RSS', col='re
d', pch=19, type='b')
```

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 $plot(\ dof_choices,\ cv.rss.test.mean,\ xlab='spline\ d.o.f.',\ ylab='Test-RSS',\ col='re\ d',\ pch=19,\ type='b'\)$



using thebs() function we choose to specify the splines degree of freedom via cross-validation. This will place the knots at the percentile points of the data with a large degrees of freedom corresponding to more knots in the domain. The test RSS seems to be minimal for the degrees of freedom equal to six.

5.4 Smoothing splines

Example: Generalized Cross-Validation

```
fossil <- read.table("fossil.dat",header=T)
plot(fossil,pch=1, main="smoothed fossil data")
# smooth.spline: Fits a cubic smoothing spline to the supplied data
ssl=smooth.spline(fossil$age,fossil$strontium.ratio)
# since both spar and df are not specified, cv=FALSE
# cv (the default is FALSE): ordinary leave-one-out (TRUE) or 'generalized' cross-val
idation (GCV) when FALSE; is used for smoothing parameter computation only when both
spar and df are not specified
ssl$df</pre>
```

```
## [1] 13.10385

ss2=smooth.spline(fossil$age,fossil$strontium.ratio,df = 4)
ss2$df
```

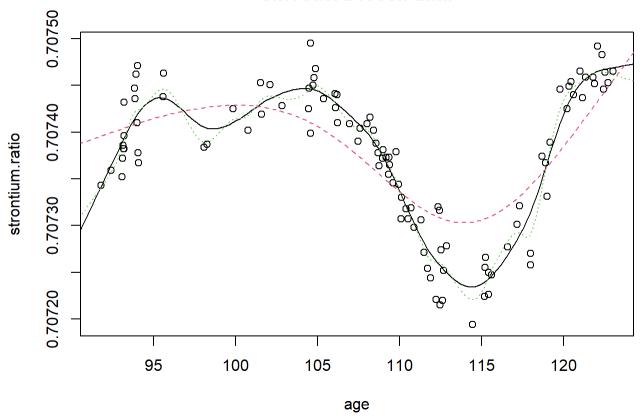
```
## [1] 3.999547
```

```
ss3=smooth.spline(fossil$age,fossil$strontium.ratio,df = 25)
ss3$df
```

```
## [1] 24.99731
```

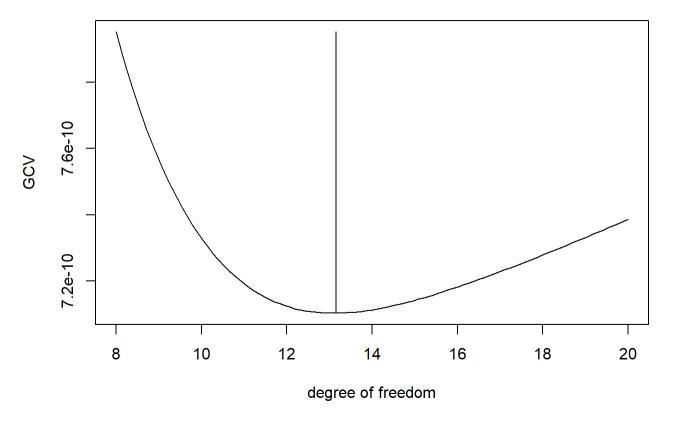
```
xx=seq(90,130,length.out = 200)
lines(predict(ss1,xx), col=1)
lines(predict(ss2,xx), col=2,lty=2)
lines(predict(ss3,xx), col=3,lty=3)
```

smoothed fossil data



The following code shows the dependence of the GCV on the d.o.f.

```
fossil <- read.table("fossil.dat",header=T)</pre>
num.df <- 101
df.grid<-seq(8,20,length=num.df)</pre>
GCV <- rep(NA,num.df)</pre>
n <- length(fossil$age)</pre>
for (i in 1:num.df)
{
 fit
        <- smooth.spline(fossil$strontium.ratio~fossil$age,df=df.grid[i])
        <- sum((fossil$strontium.ratio-predict(fit,fossil$age)$y)^2)
 RSS
 GCV[i] \leftarrow (1/n)*RSS/(1-df.grid[i]/n)^2
}
plot(df.grid,GCV,type="l",xlab="degree of freedom", ylab="GCV")
ind.min <- order(GCV)[1] #44
lines(rep(df.grid[ind.min],2),c(min(GCV),max(GCV)))
```



The same result can be obtained by simply setting cv = FALSE in smooth. spline function:

```
fossil <- read.table("fossil.dat",header=T)
sp<-smooth.spline(fossil$age,fossil$strontium.ratio,cv=FALSE)
sp$df</pre>
```

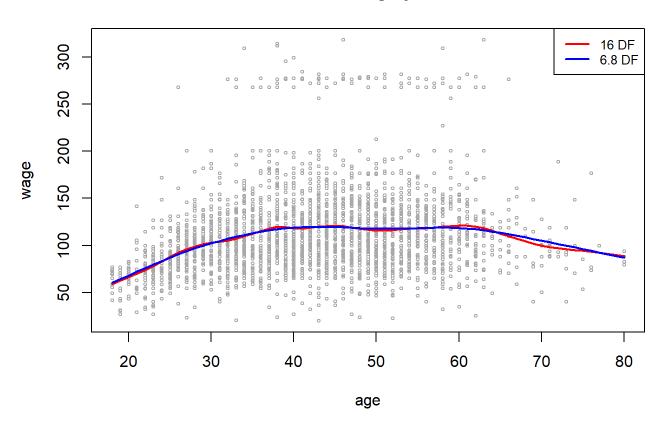
```
## [1] 13.10385
```

Activity in R: Smoothing spline

Recall the Wage data set in the library ISLR. Visualise age vs wage using a scatterplot. Fit a smoothing spline using the smooth.spline() function in R. Compare two methods of fitting the smoothing spline: one of them is by providing $\mathtt{df} = 16$ and the second one by using cross-validation $\mathtt{cv} = \mathtt{TRUE}$. Add the visualisation of both fitted splines onto the scatterplot. Explain how the fit is obtained in both cases.

```
library(ISLR)
attach(Wage)
## The following objects are masked from Wage (pos = 4):
##
##
       age, education, health, health ins, jobclass, logwage, maritl,
##
       race, region, wage, year
## The following objects are masked from Wage (pos = 8):
##
##
       age, education, health, health ins, jobclass, logwage, maritl,
       race, region, wage, year
##
## The following objects are masked from trade.union:
##
##
       age, race, wage
agelims=range(age)
plot(age,wage,xlim=agelims, cex=.5,col="darkgrey")
title("Smoothing spline")
fit=smooth.spline(age,wage,df=16)
fit2=smooth.spline(age,wage,cv=TRUE)
## Warning in smooth.spline(age, wage, cv = TRUE): cross-validation with
## non-unique 'x' values seems doubtful
fit2$df
## [1] 6.794596
lines(fit,col="red",lwd=2)
lines(fit2,col="blue",lwd=2)
legend("topright",legend=c("16 DF","6.8 DF"),col=c("red","blue"),lty=1,lwd=2,cex=.8)
```

Smoothing spline





In the first call to smooth. spline(), we specified df=16. The function then determines which λ leads to 16 degrees of freedom. In the second case, we select the smoothness level by cross-validation, and this results in a value of λ that yields df=6.8.

5.5 Multidimensional splines

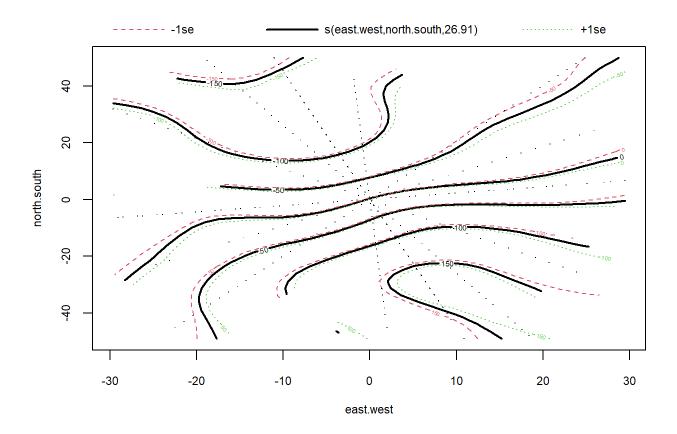
###Example: Fitting a thin plate spline in R

A thin-plate spline fit is implemented in the package mgcv:

```
require(mgcv)

## Loading required package: mgcv
```

```
## Loading required package: nlme
## This is mgcv 1.9-0. For overview type 'help("mgcv-package")'.
galaxy <-read.table("galaxy.txt")</pre>
fit=gam(formula = velocity~s(east.west,north.south),data = galaxy)
fit
##
## Family: gaussian
## Link function: identity
##
## Formula:
## velocity ~ s(east.west, north.south)
##
## Estimated degrees of freedom:
## 26.9 total = 27.91
##
## GCV score: 191.5176
plot(fit)
```



gam: Generalized additive models with integrated smoothness estimation
s(...): Function used in definition of smooth terms within gam model formula and c
ontains a list of variables that are the covariates that this smooth is a function of
#https://stats.stackexchange.com/questions/423375/why-is-there-residual-dots-in-plotof-gam

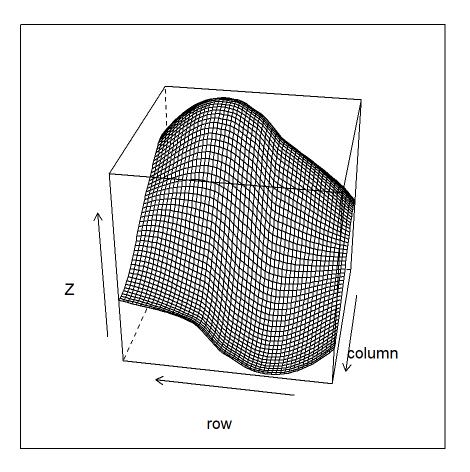
Fits in higher dimensions may be calculated as well, but are not visualised as easily. Alternatively, a loess smooth can be fitted:

##

melanoma

```
attach(galaxy)
loc.lin.reg = loess(formula = velocity ~ north.south +
                      east.west, data = galaxy, span = 0.7, degree = 2,
                    normalize = T, family = "gaussian")
xgrid = seq(min(north.south), max(north.south), length.out = 50)
ygrid = seq(min(east.west), max(east.west), length.out = 50)
new.coords = matrix(data = NA, nrow = 2500, ncol = 2)
new.coords[, 1] = as.vector(outer(rep(1, 50), xgrid))
new.coords[, 2] = as.vector(outer(ygrid, rep(1, 50)))
new.coords = as.data.frame(new.coords)
names(new.coords) <- c("north.south", "east.west")</pre>
Z = predict(loc.lin.reg, newdata = new.coords)
Z = matrix(data = Z, ncol = 50)
library(lattice)
##
## Attaching package: 'lattice'
## The following object is masked from 'package:boot':
##
```

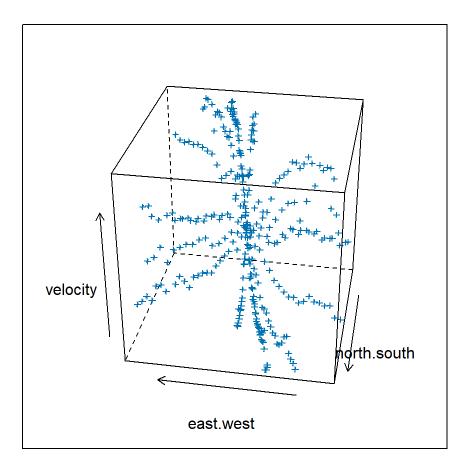
```
wireframe(Z, screen = list(z = 170, x = -60))
```



wireframe: 3d Scatter Plot and Wireframe Surface Plot

Activity in R: 3D visualisation

Consider the galaxy dataset. Generate a plot of the three-dimensional point cloud east. west, north. south, velocity using the cloud() function in the lattice library in R.



5.6 Activities

In this exercise we follow the Lab notes from Section 7.8 of James et al. (2013), i.e. the ISLR book. We will skip Section 7.8.1 on polynomial regression and step functions but it is recommended to read through this section (combined with the course notes). Instead we focus on section 7.8.2 to learn how to fit regression splines, natural splines and smoothing splines.

We will focus on the Wage dataset available in the R package ISLR.

• Consider a spline regression to fit wage to age considering knots at 25, 40 and 60. Represent the estimated regression line for a sequence of age values of length 100 ranging from the minimum to the maximum observed values. Add a confidence interval using ±2 standard error.

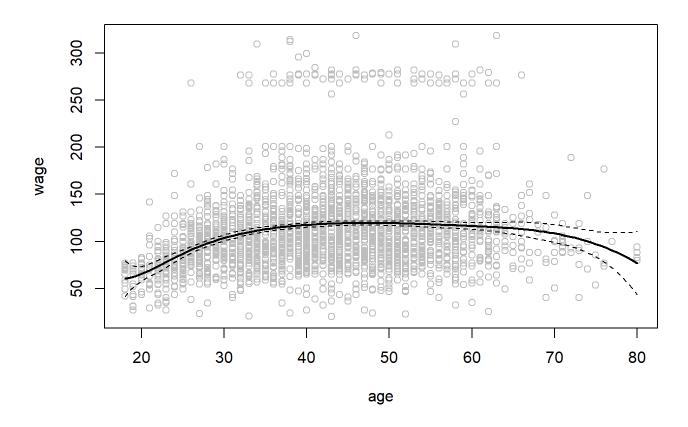
```
library(ISLR)

data("Wage")
attach(Wage)

## The following objects are masked from Wage (pos = 7):
##

## age, education, health, health_ins, jobclass, logwage, maritl,
## race, region, wage, year
```

```
## The following objects are masked from Wage (pos = 9):
##
       age, education, health, health ins, jobclass, logwage, maritl,
##
##
       race, region, wage, year
## The following objects are masked from Wage (pos = 13):
##
##
       age, education, health, health ins, jobclass, logwage, maritl,
##
       race, region, wage, year
## The following objects are masked from trade.union:
##
##
       age, race, wage
fit <- lm(wage~bs(age, knots=c(25,40,60)), data=Wage)</pre>
age.grid <- seq(from=min(age), to=max(age), length=100)</pre>
pred <- predict(fit, newdata=list(age=age.grid), se=TRUE)</pre>
plot(age, wage, col="gray")
lines(age.grid, pred$fit, lwd=2)
lines(age.grid, pred$fit + 2*pred$se, lty=2)
lines(age.grid, pred$fit - 2*pred$se, lty=2)
```



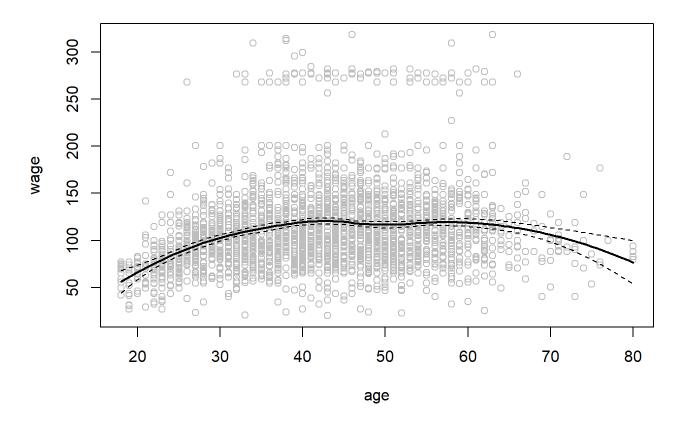
• How many basis function were used in the previous question? Now, instead of specifying the locations of the knots, use the df and degree arguments to specify a quadratic spline regression with 6 degrees of freedom. Fit the model and display it as in 1). Where were the knots located?

```
fit2 <- lm(wage~bs(age, df=6, degree=2), data=Wage)
attr(bs(age, df=6, degree=2), "knots")</pre>
```

```
## [1] 32 39 46 53
```

```
# 20% 40% 60% 80%
# 32 39 46 53
pred2 <- predict(fit2, newdata=list(age=age.grid), se=TRUE)

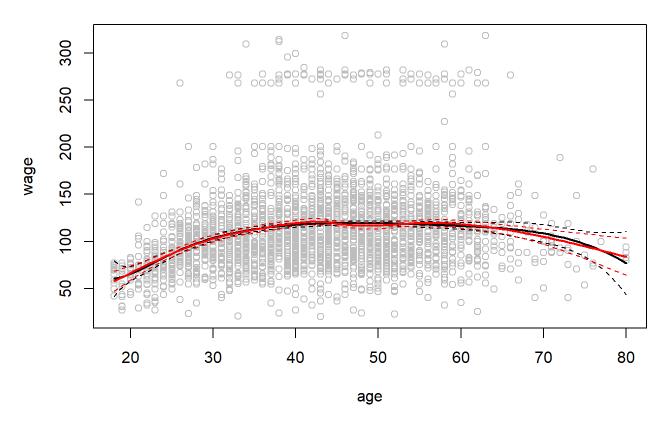
plot(age, wage, col="gray")
lines(age.grid, pred2$fit, lwd=2)
lines(age.grid, pred2$fit + 2*pred2$se, lty=2)
lines(age.grid, pred2$fit - 2*pred2$se, lty=2)</pre>
```



• Use the ns() function to fit a natural cubic spline with 6 degree of freedom. Superimpose it with the spline regression from 1). What is the main comment that you can make when comparing both models?

```
fit3 <- lm(wage~ns(age, df=6), data=Wage)
pred3 <- predict(fit3, newdata=list(age=age.grid), se=TRUE)

plot(age, wage, col="gray")
lines(age.grid, pred$fit, lwd=2)
lines(age.grid, pred$fit + 2*pred$se, lty=2)
lines(age.grid, pred$fit - 2*pred$se, lty=2)
lines(age.grid, pred3$fit, lwd=2, col="red")
lines(age.grid, pred3$fit + 2*pred3$se, lty=2, col="red")
lines(age.grid, pred3$fit - 2*pred3$se, lty=2, col="red")</pre>
```



We observe less variability at the boundary of the support when using the natural splines.

• Use the smooth. spline() function to fit a smoothing spline to the data. In the first place use the argument df = 16 allowing for a 16 degrees of freedom. In a second step, consider instead the argument cv = TRUE to use cross-validation to select the optimal degree of freedom. Display both fitted lines. What do the respective models do?

```
plot(age, wage, xlim=range(age), cex=0.5, col="darkgrey")
title("Smoothing Spline")
fit4 <- smooth.spline(age, wage, df=16)
fit5 <- smooth.spline(age, wage, cv=TRUE)

## Warning in smooth.spline(age, wage, cv = TRUE): cross-validation with
## non-unique 'x' values seems doubtful</pre>
table(age)
```

```
## age
##
    18
         19
              20
                  21
                       22
                            23
                                 24
                                      25
                                           26
                                                27
                                                    28
                                                         29
                                                              30
                                                                   31
                                                                        32
                                                                             33
                                                                                  34
                                                                                      35
                                                                                           36
                                                                                                37
                                      56
                                                         58
                                                                        78
##
    11
         14
              20
                   15
                       38
                            45
                                 32
                                           47
                                                53
                                                    59
                                                              74
                                                                   63
                                                                             87
                                                                                  76
                                                                                      75
                                                                                           66
                                                                                                77
##
    38
         39
              40
                   41
                       42
                            43
                                 44
                                      45
                                           46
                                                47
                                                    48
                                                         49
                                                              50
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                                                                                           56
                                                                                                57
         89 113
                  92
                       88
                            98
                                 93
                                      95
                                                98
                                                    93
                                                         83
                                                              95
                                                                   82
                                                                        69
                                                                             62
                                                                                  68
                                                                                                42
##
    83
                                           80
                                                                                      65
                                                                                           62
##
    58
         59
              60
                   61
                       62
                            63
                                 64
                                      65
                                           66
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                                                    68
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                                                                             73
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                                                                                                77
                                                           5
                                                               6
                                                                    8
                                                                         3
                                                                              5
                                                                                   3
                                                                                        2
                                                                                            3
                            27
                                 11
                                       8
                                           13
                                                 7
                                                      4
                                                                                                 1
##
    57
         39
              37
                   33
                       30
##
    80
     4
##
```

fit5\$df

```
## [1] 6.794596
```

```
lines(fit4, col="red", lwd=2)
lines(fit5, col="blue", lwd=2)
```

Smoothing Spline

