Model Free Curve Fitting

- Response variable: Y
- Explanatory variables

$$X_1, X_2, \ldots, X_p$$

- Summarize or describe trends in the conditional mean of Y.
  - No model is specified
  - Fit a "smooth" curve

Applications

- Fitting a smooth curve to a plot can be a first step in building a parametric model
  - Roughly determine the "shape" of the curve
  - Little subject matter motivation
  - No need to specify a parametric formula

$$Y_i = \underline{\beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \epsilon_i}$$

  - Let the data speak for themselves.

- Check the fit of a parametric model

- Make predictions (interpolation)

  Must store $\begin{matrix} X_1 & \widehat{Y}_1 \\ X_2 & \widehat{Y}_2 \\ \vdots & \vdots \\ X_k & \widehat{Y}_k \end{matrix}$

  Use linear interpolation?

- Extrapolation?

Diabetes data: (Sockett, et al. 1987)

- Factors affecting patterns of insulin-dependent diabetes mellitus in children.

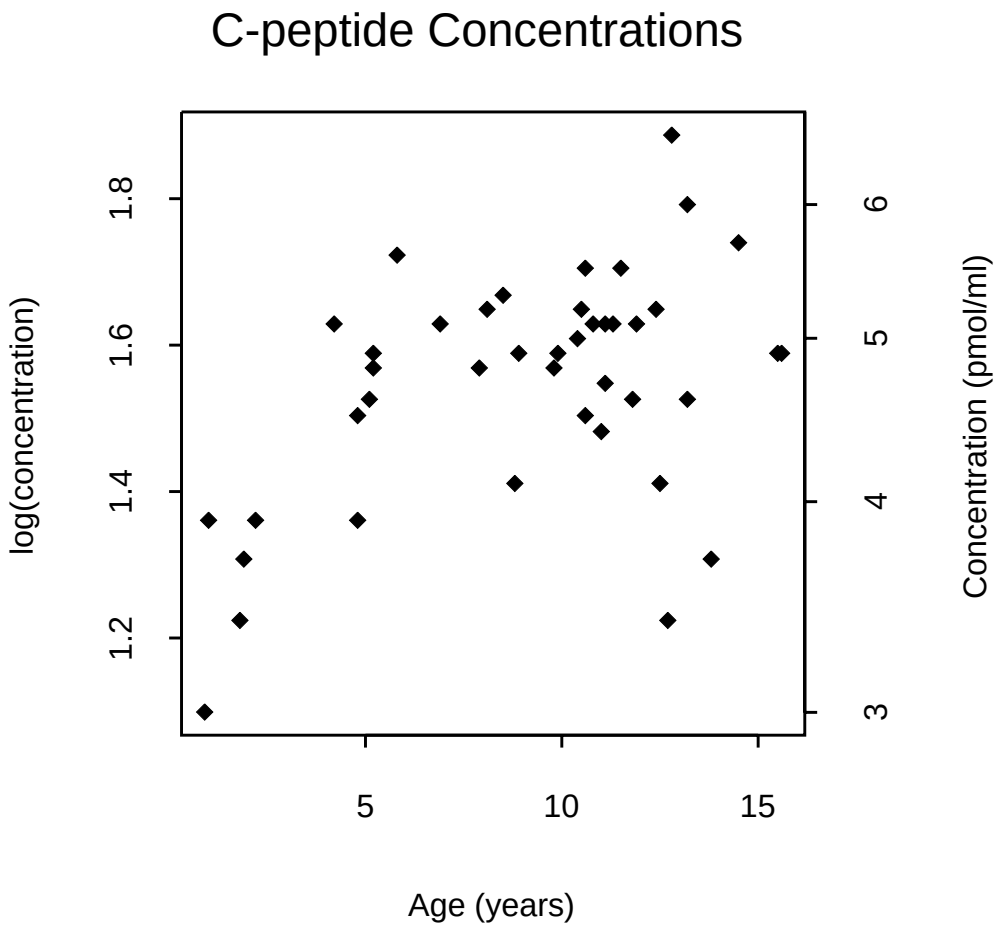
- Level of serum C-peptide at diagnosis

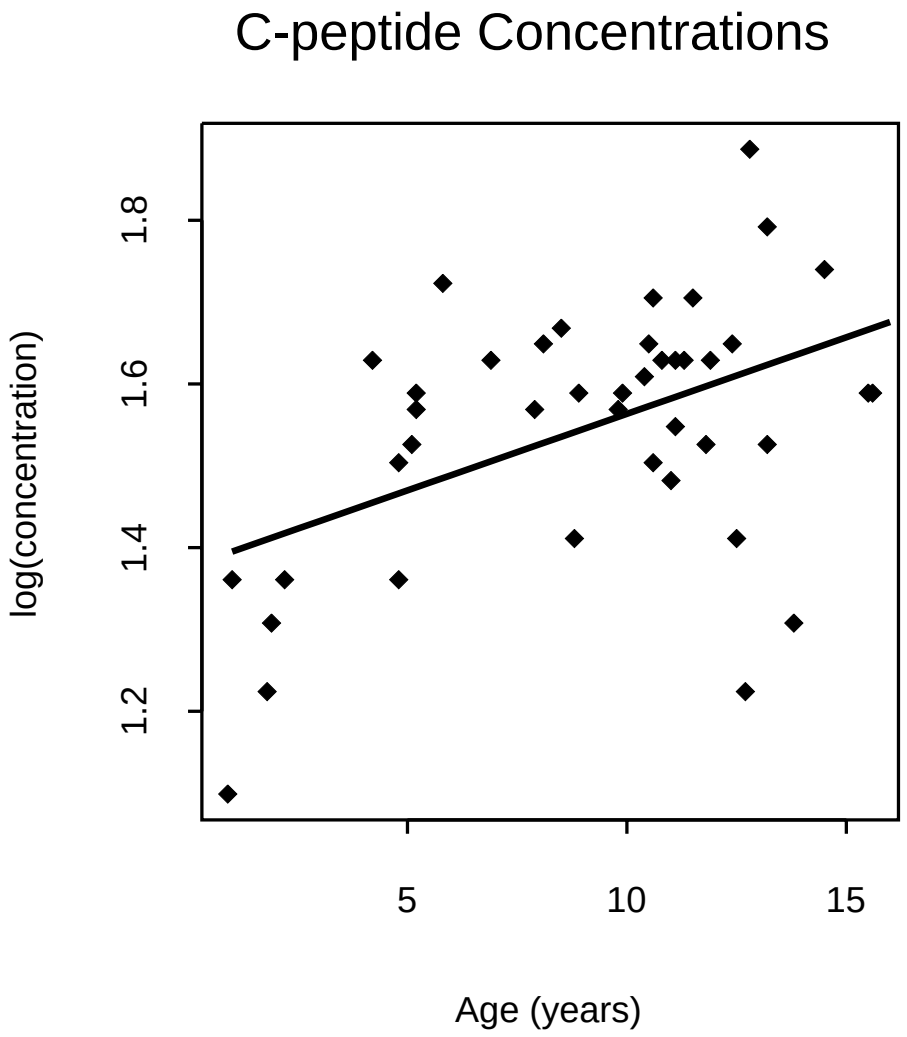
  $Y =$ log (serum C-peptide conc.)

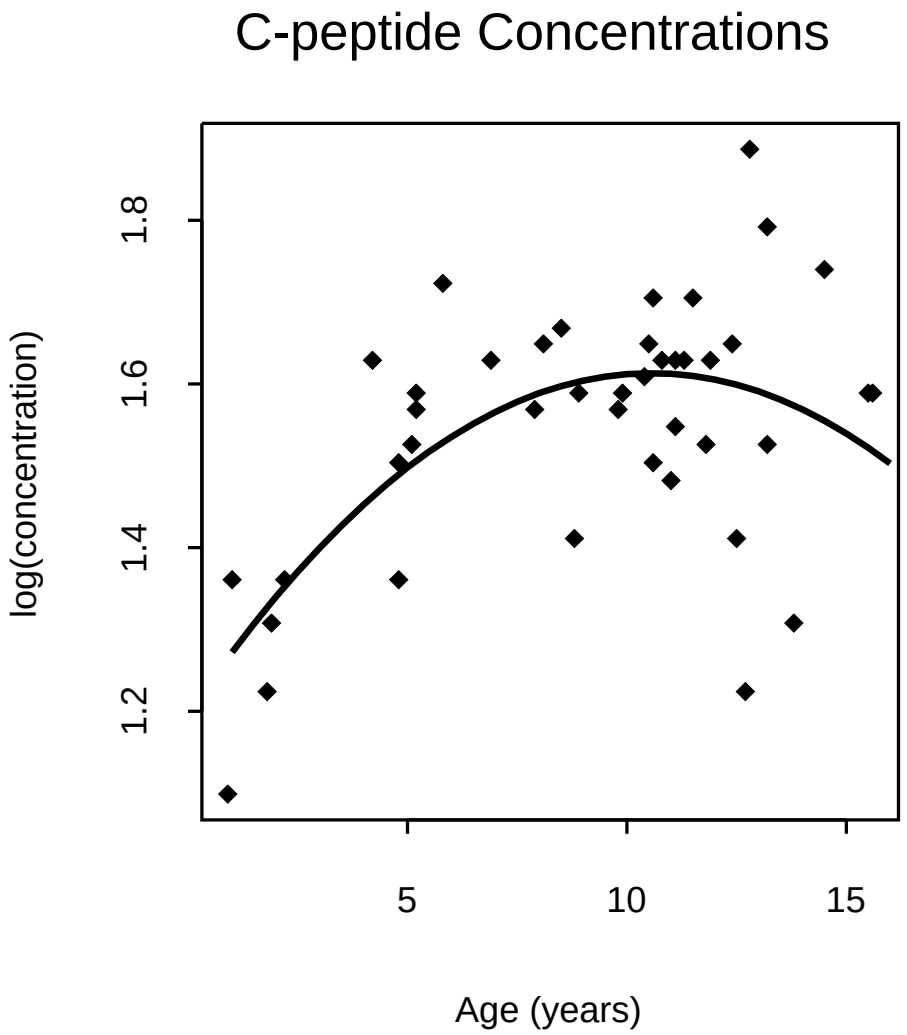
- $X =$ age (in years) at diagnosis.

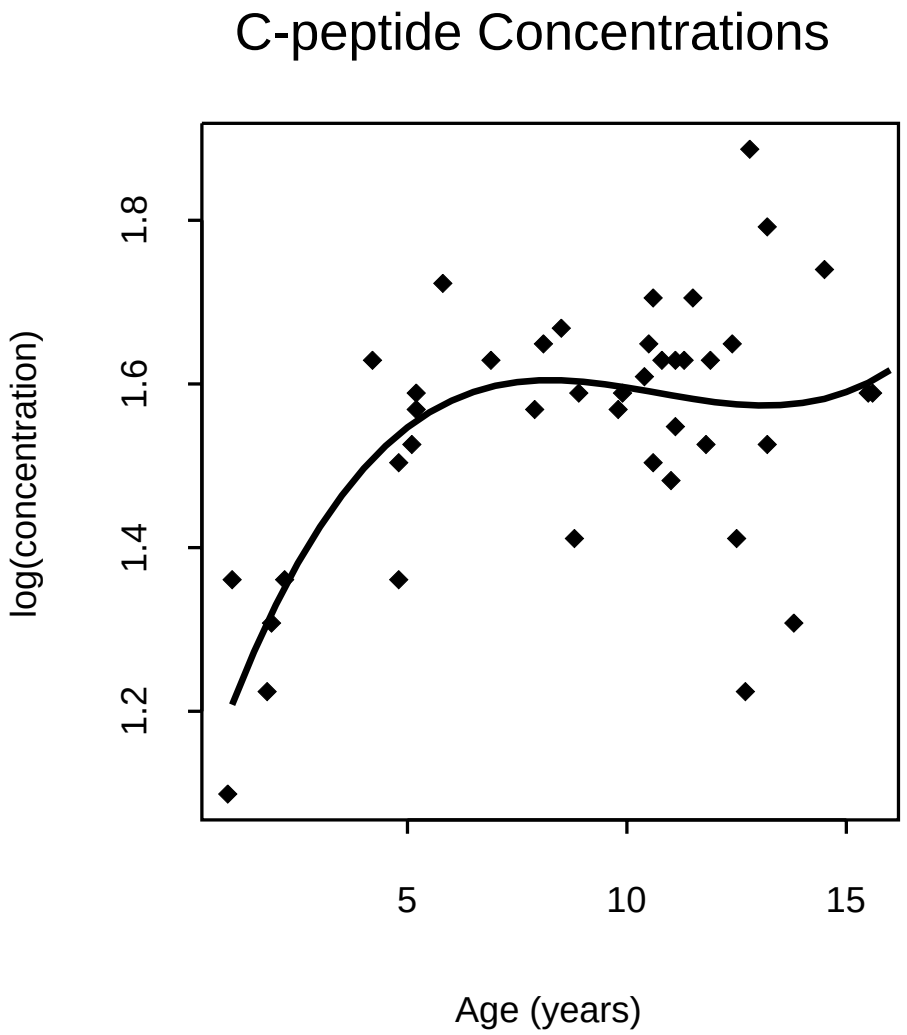
subject	age	basedef	Cpeptide	Y
15	0.9	-11.6	3.0	1.099
24	1.0	-8.2	3.9	1.361
6	1.8	-19.2	3.4	1.224
10	1.9	-25.0	3.7	1.308
11	2.2	-3.1	3.9	1.361
36	4.2	-17.0	5.1	1.629
12	4.8	-7.8	4.5	1.504
35	4.8	-9.5	3.9	1.361
34	5.1	-5.1	4.6	1.526
1	5.2	-8.1	4.8	1.569
14	5.2	-4.5	4.9	1.589
9	5.8	-2.8	5.6	1.723
37	6.9	-3.3	5.1	1.629
13	7.9	-13.9	4.8	1.569
17	7.9	-2.0	4.8	1.569
27	8.1	-1.6	5.2	1.649
20	8.5	-0.2	5.3	1.668
2	8.8	-16.1	4.1	1.411
42	8.9	-10.0	4.9	1.589
30	9.8	-1.2	4.8	1.569
39	9.9	-3.3	4.9	1.589

subject	age	basedef	cpeptide	Y
5	10.4	-29.0	5.0	1.609
3	10.5	-0.9	5.2	1.649
4	10.6	-7.8	5.5	1.705
19	10.6	-11.2	4.5	1.504
43	10.8	-13.5	5.1	1.629
31	11.0	-14.3	4.4	1.482
21	11.1	-6.1	4.7	1.548
33	11.1	-16.8	5.1	1.629
23	11.3	-3.6	5.1	1.629
18	11.5	-9.0	5.5	1.705
16	11.8	-2.1	4.6	1.526
26	11.9	-2.0	5.1	1.629
32	12.4	-0.8	5.2	1.649
40	12.5	-13.6	4.1	1.411
7	12.7	-18.9	3.4	1.224
22	12.8	-1.0	6.6	1.887
38	13.2	-0.7	6.0	1.792
41	13.2	-1.9	4.6	1.526
28	13.8	-11.9	3.7	1.308
25	14.5	-0.5	5.7	1.740
29	15.5	-0.7	4.9	1.589
8	15.6	-10.6	4.9	1.589


C-peptide Concentrations
log(concentration)
1.2
1.4
1.6
1.8
Concentration (pmol/ml)
3
4
5
6
5
10
15
Age (years)


C-peptide Concentrations
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)


C-peptide Concentrations
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)


C-peptide Concentrations
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)

```
# This is SPLUS code for plotting
# log(C-peptide concentration)
# against age. This file stored as
#         cpeptide1.spl

# The data are stored in the file
#         cpeptide.tex

# There are four numbers on each line
# in the following order:
#      Subject identification code
#      Age at diagnosis (years)
#      Base deficit (measure of acidity)
#      C-peptide concentration (pmol/ml)
# Enter the data into a data frame
# Compute the natural log of the
# C-peptide concentration.

cpep <- read.table("cpeptide.tex", header=T)
cpep$Y <- log(cpep$Cpeptide)
cpep$Y <- round(cpep$Y,digits=3)
```

```
#  Sort the data file by age

i <- sort.list(cpep$age)
cpep <- cpep[i,]
cpep

# Code for plotting weight against time
# Specify plotting symbol and size of
# graph in inches.
#   fin=c(w,h) specifies a plot that is w
#         inches wide and h inches high.
# pch=18  requests a filled diamond as a
#         plotting symbol.
# mkh=b   requests plotting symbols that
#         are  b  inches high.
# mex=a   sets the spacing between lines
#         printed in the margins.
# plt     plt=c(.2,.8,.2,.8) defines the
#         fraction of figure region to use
#         for plotting.  This can provide
#         more space for to label margins.
```

```
par(fin=c(7.0,7.0),pch=18,mkh=.1,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="p",
       xlab="Age (years)",
       ylab="log(concentration)",
       main="C-peptide Concentrations")


# The following three lines are for adding
# an axis for C-peptide concentration on
# the original scale (pmol/ml).
# pretty(): Returns a vector of ordered
# and equally spaced values that span
# the range of the input.

Y.exp <- pretty(range(exp(cpep$Y)))
  axis(side=4, at=log(Y.exp),
               lab=Y.exp, srt=90)
  mtext("Concentration (pmol/ml)",
               side=4, line=3)
```

```
# Fit a  straight line model

cpep.lin <- lm(Y~age,data=cpep)


par(fin=c(7.0,7.0),pch=18,mkh=.1,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="p",
       xlab="Age (years)",
       ylab="log(concentration)",
       main="C-peptide Concentrations")
a <- seq(1, 16, .5)
lines(a, predict(cpep.lin, data.frame(age=a),
        type="response"),lty=1,lwd=3)
```

```
# Fit a quadratic model

cpep.q <- lm(Y~age+age^2,data=cpep)

par(fin=c(7.0,7.0),pch=18,mkh=.1,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="p",
       xlab="Age (years)",
       ylab="log(concentration)",
       main="C-peptide Concentrations")
a <- seq(1, 16, .5)
lines(a, predict(cpep.q, data.frame(age=a),
        type="response"),lty=1,lwd=3)
```

```
# Fit a cubic model

cpep.3 <- lm(Y~age+age^2+age^3,data=cpep)

par(fin=c(7.0,7.0),pch=18,mkh=.1,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="p",
       xlab="Age (years)",
       ylab="log(concentration)",
       main="C-peptide Concentrations")
a <- seq(1, 16, .5)
lines(a, predict(cpep.3, data.frame(age=a),
        type="response"),lty=1,lwd=3)
```

"Bin" Smoothers:

- Partition the range of the explanatory variable (X) into p disjoint and exhaustive regions

- About the same number of observations in each "bin"
- Compute the average of the responses (Y values) in each bin

Running mean or median smoothers

- Use a different "bin" for each value of the explanatory variable X
- **Symmetric nearest neighbor version:** Find the nearest k cases to the left of X and the nearest k cases to the right of X
  - Compute the mean (or median)
  - Include X?
  - Boundary considerations
- **Nearest neighbor version:** Use the r nearest cases to X

Running mean or median smoothers

- Simple to compute
- May not be smooth enough
- Tend to flatten out trends near the boundaries)

Running Line Smoothers

- Fit a least squares regression line to the points "near" X
  - Symmetric nearest neighbors
  - Nearest neighbors

- Predict the mean response at X

$$\hat{Y}_X = b_{0,X} + b_{1,X}X$$

↗ ↗

The estimated coefficents will not be the same for every X
(local regression lines)

- parbox[t]6.0inUsing larger neighborhoods produces smoother curves.

Running Line Smoothers

- In the center of the data
  - the intercept is dominant
  - the slope plays a smaller role
- Near the edges (boundaries)
  - Slope is important for picking up trends in asymmetric neighborhoods of X.
  - This reduces some of the "bias" associated with running means.

- Points inside a neighborhood have equal weight.
  - points "outside" have zero weight
  - source of jaggedness
  - "weight" the points in a neighorhood.
    * higher weights for points closer to X.
    * weights go to zero near the ends of the neighborhood.
  - Cleveland's "loess" smoother

Kernel Smoothers

- Local weighted average with local weights defined by a "kernel".

$$\widehat{Y}_i = \frac{\sum_{j=1}^{n} Y_j K\left(\frac{X_j - X}{b}\right)}{\sum_{j=1}^{n} K\left(\frac{X_j - X}{b}\right)}$$

- the value of $K\left(\frac{X_j - X}{b}\right)$ decreases in a "smooth" way as X_j moves farther away from X.

- b is the "bandwidth".

Examples:

"Gausian" kernel smoother

$$K\left(\frac{X_j - X}{b}\right) = \frac{1}{\sqrt{2\pi}\, b} e^{\frac{1}{2}(\frac{X_j - X}{b})^2}$$

"Minimum variance" kernel

$$K(\frac{X_j - X}{b}) = \begin{cases} \frac{3}{8b}(3 - 5[\frac{X_j - X}{b}]^2) \\ \qquad \text{if} \quad |\frac{X_j - X}{b}| < 1 \\ 0 \quad \text{otherwise} \end{cases}$$

This choice of weights minimizes the large sample variance of the estimator.

- The "kernel" is truncated at the end of the data.

- Simulation studies have shown that
  - the choice of the form of the kernel is not very important.
  - the "bandwidth" is important.

Locally Weighted Running Line Smoothers (loess)

Data:

$$\begin{array}{cc} (X_1 & Y_1) \\ (X_2 & Y_2) \\ \vdots & \vdots \\ (X_n & Y_n) \end{array}$$

Objective:

Estimate the conditional means of Y at a set of X values.

- Use cases in a neighborhood of X
- Fit a regression model
- Use weighted least squares estimation

(Step 1) Identify the k observations with X_j values closest to X

Identify this set of k nearest neighbors as $N_k(X)$.

(Step 2) Compute the distance of the farthest near neighbor

$$\Delta_K(X) = \max_{X_j \, \epsilon \, N_K(X)} |X - X_j|$$

(Step 3) Assign weights to each of the "near" neighbors using the tricube weight funct4ion

$$W_j = W\left(\frac{|X - X_j|}{\Delta_k(X)}\right).$$

where

$$W(u) = \begin{cases} (1-u^3)^3, & 0 \le u < 1 \\ 0, & \text{otherwise} \end{cases}$$

(Step 4) Fit a regression line using weighted least squares.

Find a_X and b_X to minimize

$$\sum_{j=1}^{n} W_j(Y_j - a_X - b_X X_j)^2$$

Solution:

$$b_X = \frac{\sum_{j=1}^{n} W_j(X_j - \bar{X})(Y_j - \bar{Y}_X)}{\sum_{j=1}^{n} W_j(X_j - \bar{X})^2}$$

$$a_X = \bar{Y}_X - b_X \bar{X}$$

where

$$\bar{X} = \frac{\sum_{j=1}^{n} W_j X_j}{\sum_{j=1}^{n} W_j}$$

$$\bar{Y} = \frac{\sum_{j=1}^{n} W_j Y_j}{\sum_{j=1}^{n} W_j}$$

(Step 5) Predict at X:

$$\hat{Y}_X = a_X + b_X(X)$$

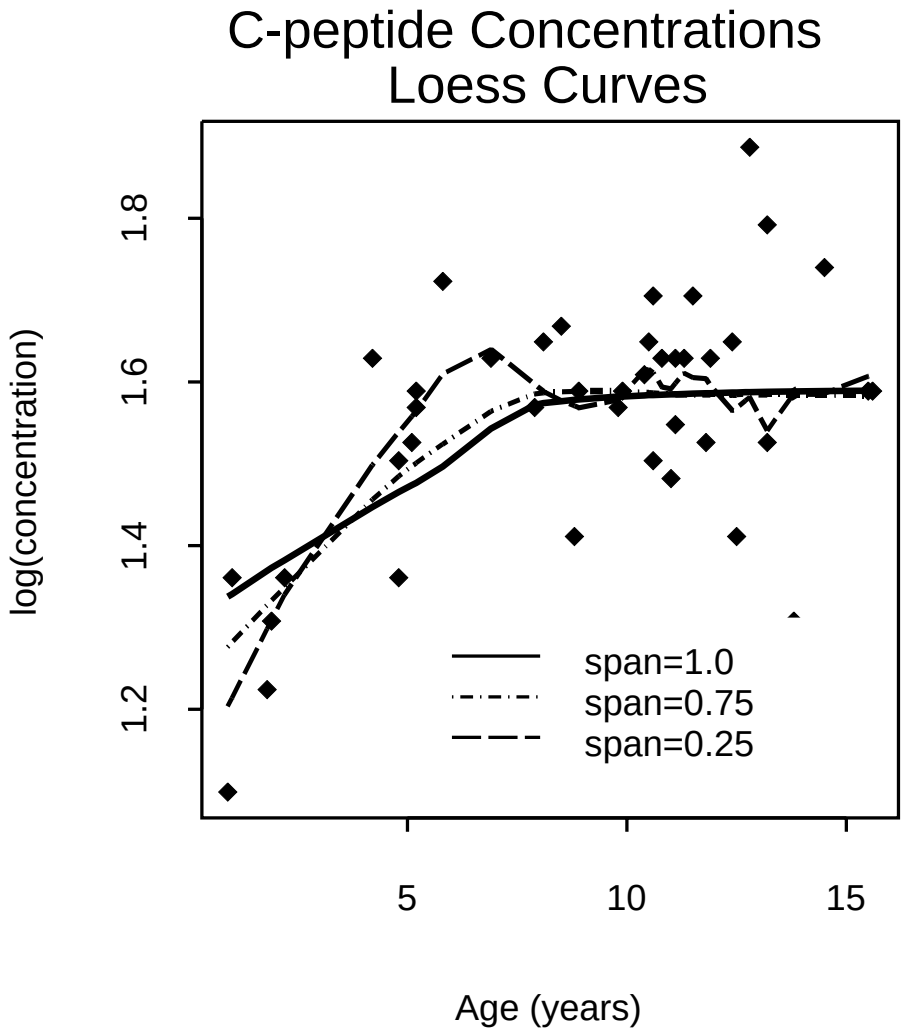
and record $(X, \hat{Y}_X)$

Repeat Steps 1 to 5 for a series of X values:

- You could fit local polynomial regression curves.

$$\widehat{Y}_X = a_X + b_X X + c_X X^2$$

- You could replace the tri-cube weight function.
- The size of $N_K(X)$ is important.


C-peptide Concentrations
Loess Curves
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)
span=1.0
span=0.75
span=0.25

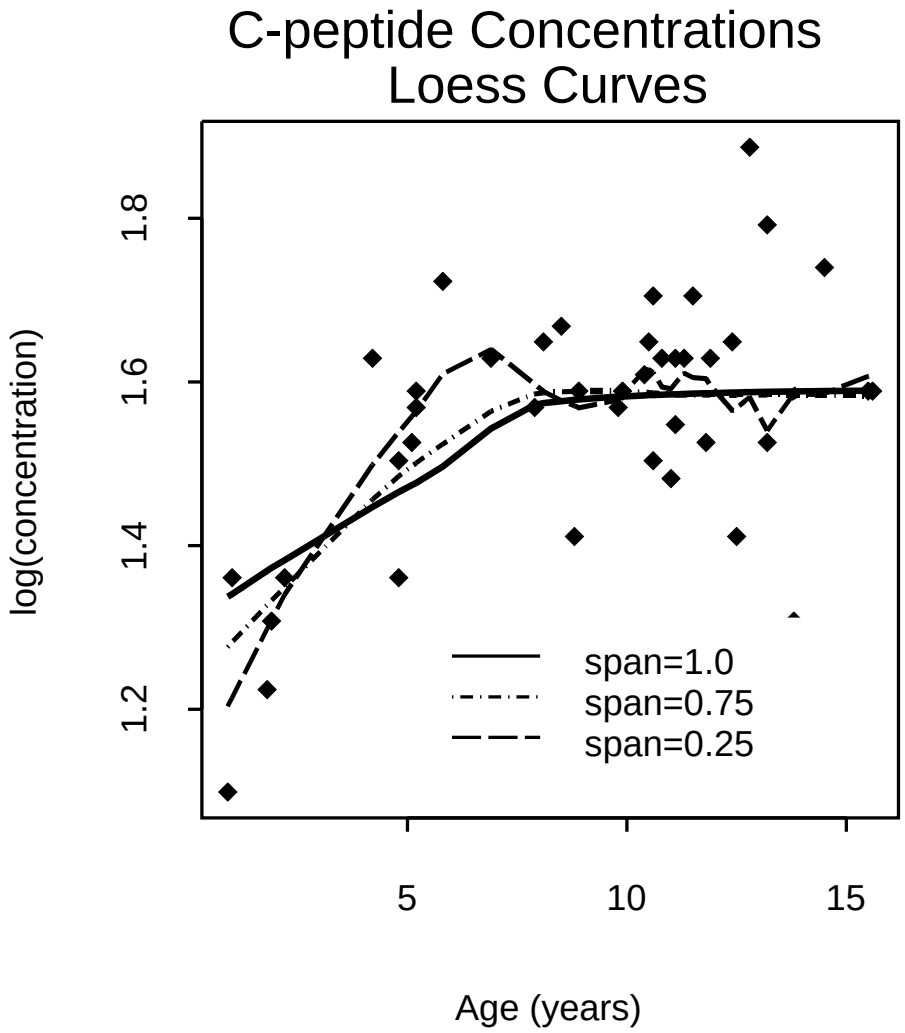
How wide should your local neighorhoods be?

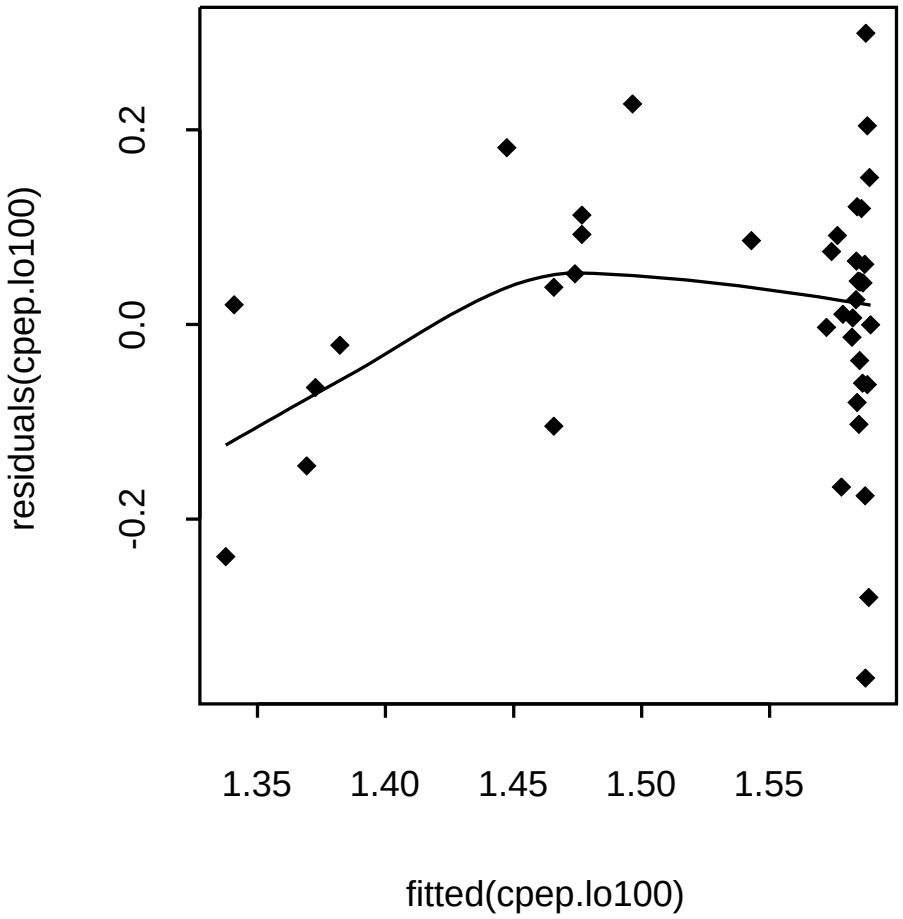
- Small
  - curve is less smooth (increase variability)
  - react to local changes (reduce bias)
- Large
  - curve is smoother (less variability)
  - may "smooth out" local patterns (more bias).

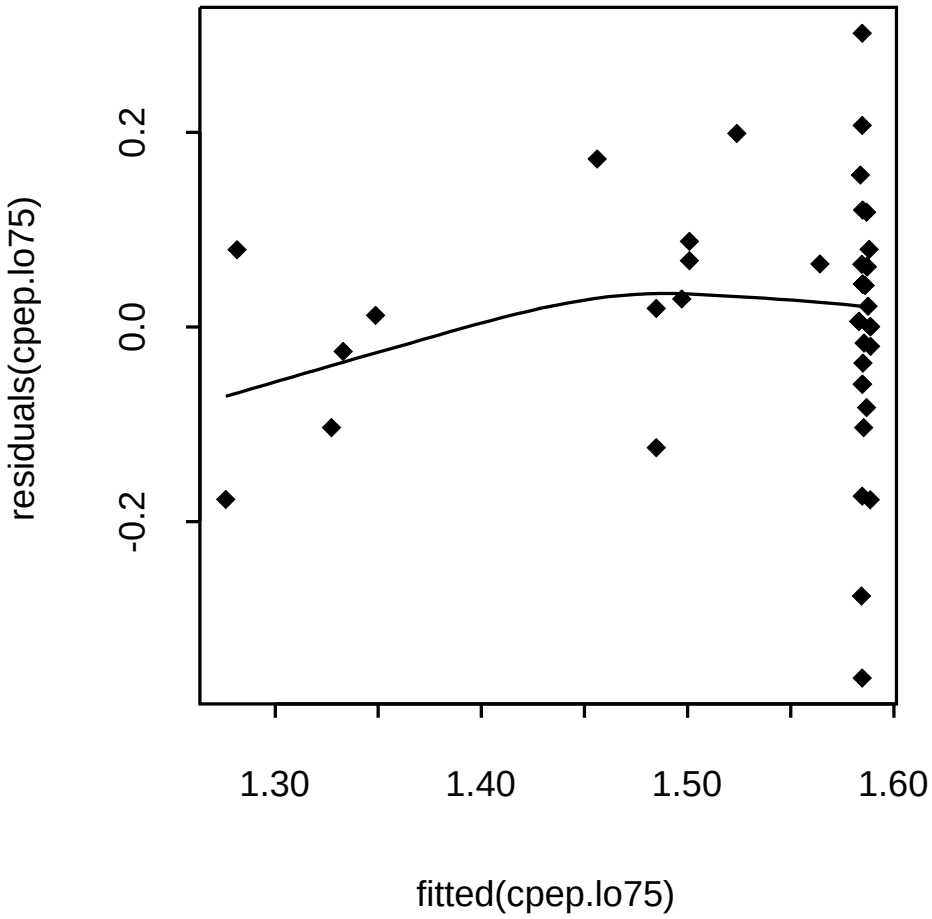
```
> #  Compare the loess curves with different spans
>
>  cpep.lo100 <- loess(formula=Y~age,
                       data=cpep,span=1.00,degree=1)
>  cpep.lo75 <- loess(formula=Y~age,
                       data=cpep,span=.75,degree=1)
>  cpep.lo25 <- loess(formula=Y~age,
                       data=cpep,span=.25,degree=1)
>
>  anova(cpep.lo100,cpep.lo75,cpep.lo25)


Model 1:
loess(formula = Y ~ age, data = cpep,
                         span = 1, degree = 1)
Model 2:
loess(formula = Y ~ age, data = cpep,
                       span = 0.75, degree = 1)
Model 3:
loess(formula = Y ~ age, data = cpep,
                       span = 0.25, degree = 1)
```

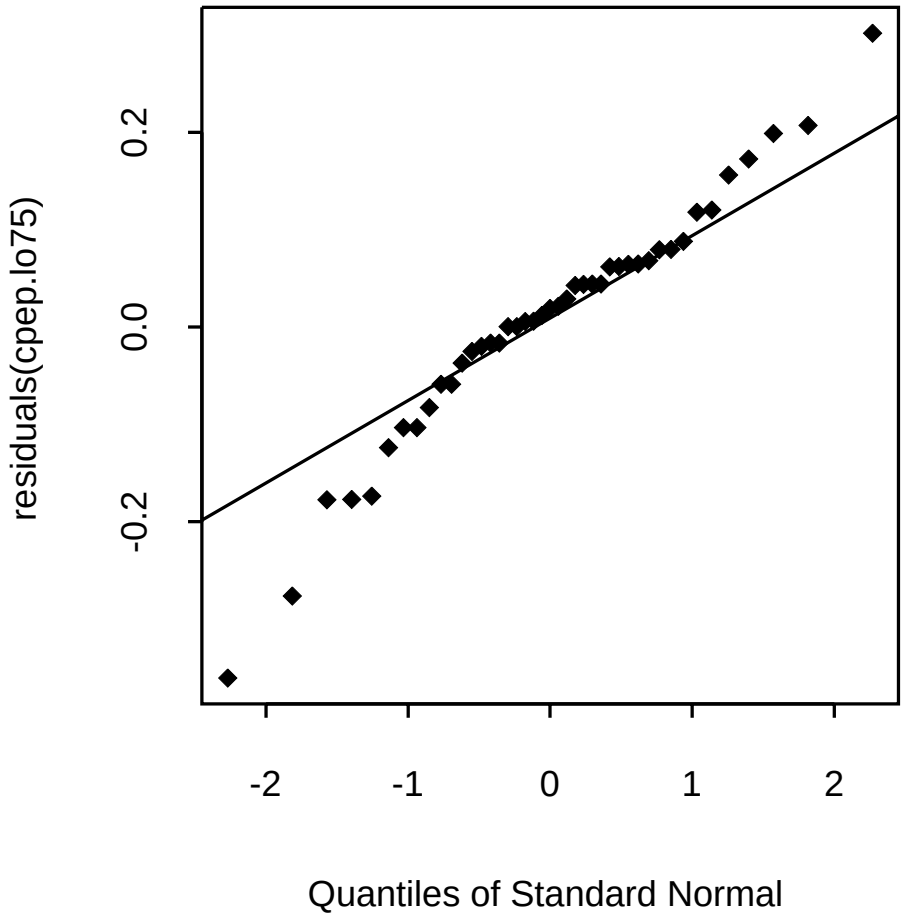
```
Analysis of Variance Table
      ENP     RSS     Test  F Value     Pr(F)
1     2.3 0.72033   1 vs 2     2.88  0.098068
2     2.9 0.66027   2 vs 3     0.31  0.951810
3     8.5 0.61296
```

```
# Plot residuals

scatter.smooth(fitted(cpep.lo100),
 residuals(cpep.lo100), span=1, degree=1)
scatter.smooth(fitted(cpep.lo75),
 residuals(cpep.lo75), span=1, degree=1)
scatter.smooth(fitted(cpep.lo25),
 residuals(cpep.lo25), span=1, degree=1)

qqnorm(residuals(cpep.lo75))
qqline(residuals(cpep.lo75))
```

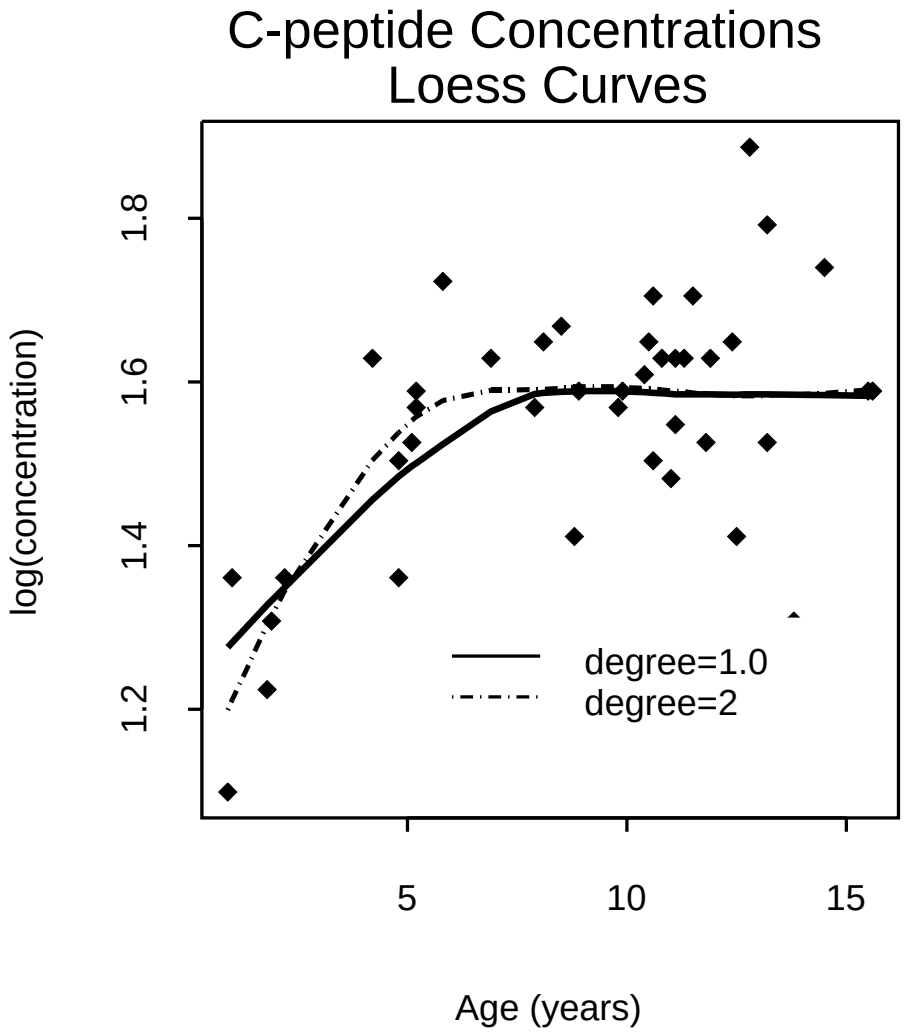

C-peptide Concentrations
Loess Curves
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)
span=1.0
span=0.75
span=0.25


residuals(cpep.lo100)
0.2
0.0
-0.2
1.35
1.40
1.45
1.50
1.55
fitted(cpep.lo100)

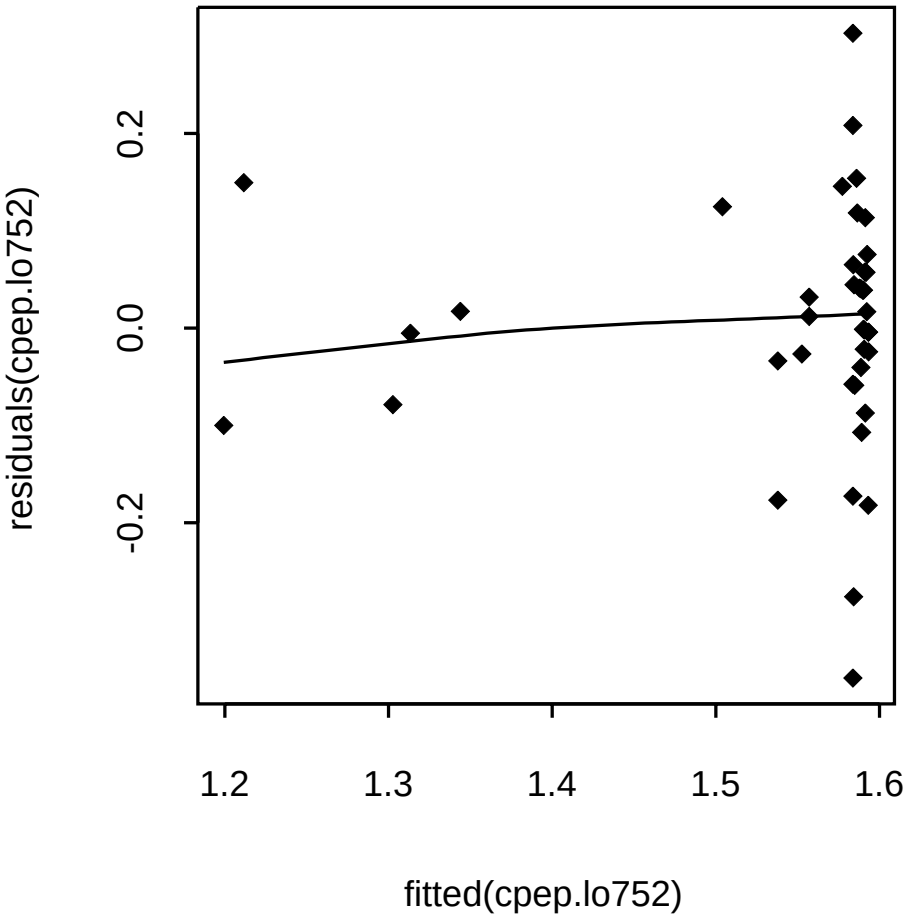

residuals(cpep.lo75)
0.2
0.0
-0.2
1.30
1.40
1.50
1.60
fitted(cpep.lo75)

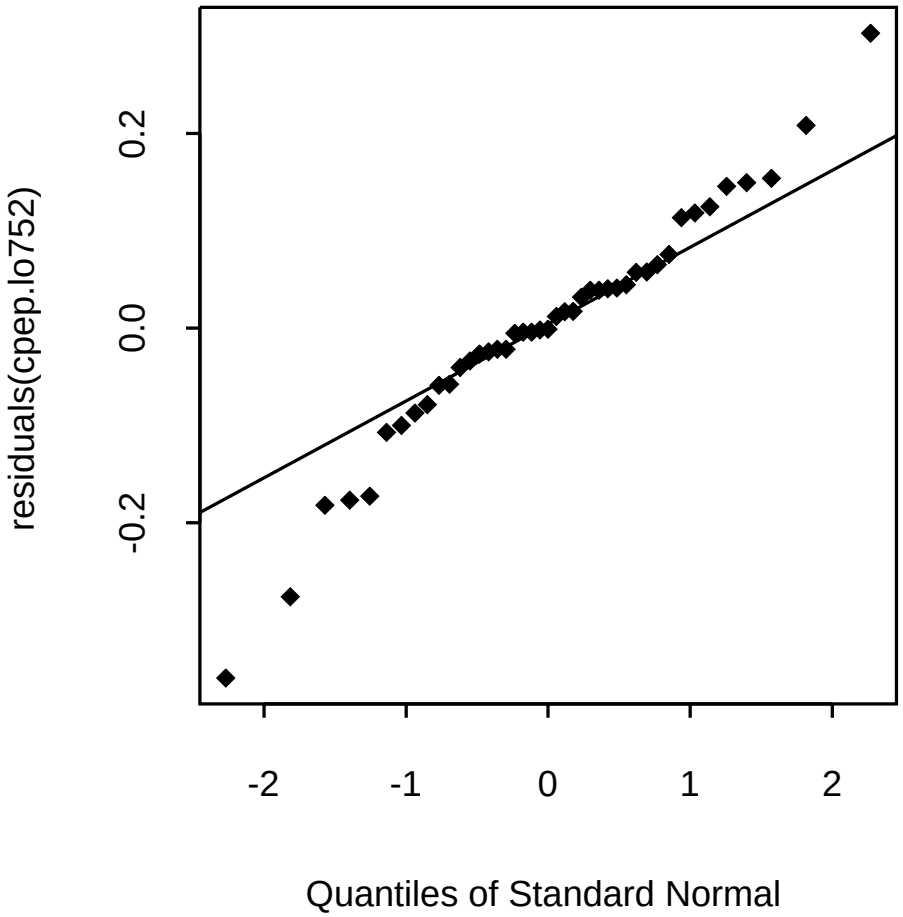

residuals(cpep.lo75)
0.2
0.0
-0.2
-2
-1
0
1
2
Quantiles of Standard Normal

```
#  Consider a second degree polynomial smoother

par(fin=c(7.0,7.0),pch=18,mkh=.1,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="p",
  xlab="Age (years)",
  ylab="log(concentration)",
  main="C-peptide Concentrations \n Loess Curves")
lines(cpep$age, loess(formula=Y~age,data=cpep,
  span=.75,degree=1)$fitted.values, lty=1,lwd=3)
lines(cpep$age, loess(formula=Y~age,data=cpep,
  span=.75,degree=2)$fitted.values, lty=3,lwd=3)
legend(5,1.31,c("degree=1.0", "degree=2"),
       lty=c(1,3),bty="n")
```


C-peptide Concentrations
Loess Curves
log(concentration)
1.2
1.4
1.6
1.8
5
10
15
Age (years)
degree=1.0
degree=2

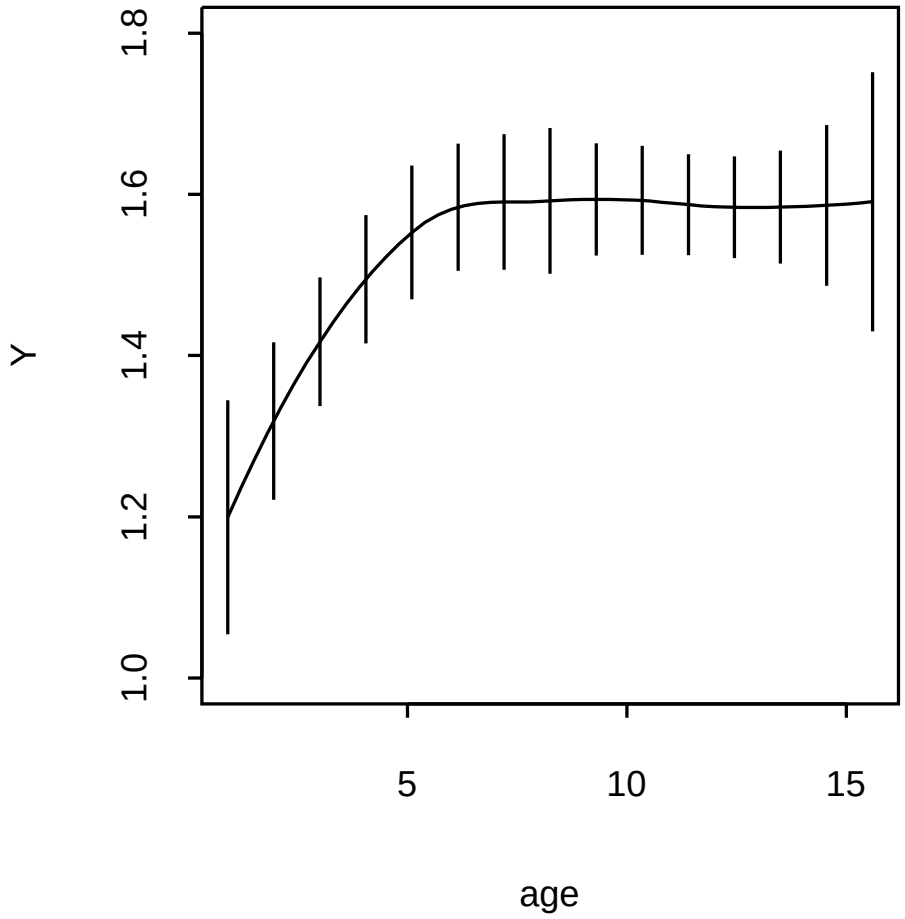
```
 cpep.lo751 <- loess(formula=Y~age,
        data=cpep,span=.75,degree=1)
 cpep.lo752 <- loess(formula=Y~age,
        data=cpep,span=.75,degree=2)

 anova(cpep.lo751,cpep.lo752)

Model 1:
loess(formula = Y ~ age, data = cpep,
        span = 0.75, degree = 1)
Model 2:
loess(formula = Y ~ age, data = cpep,
        span = 0.75, degree = 2)

Analysis of Variance Table
      ENP     RSS     Test  F Value    Pr(F)
1     2.9 0.66027   1 vs 2    1.54   0.22873
2     4.6 0.61928

# Plot residuals

scatter.smooth(fitted(cpep.lo752),
  residuals(cpep.lo752), span=1, degree=1)

qqnorm(residuals(cpep.lo752))
qqline(residuals(cpep.lo752))
```

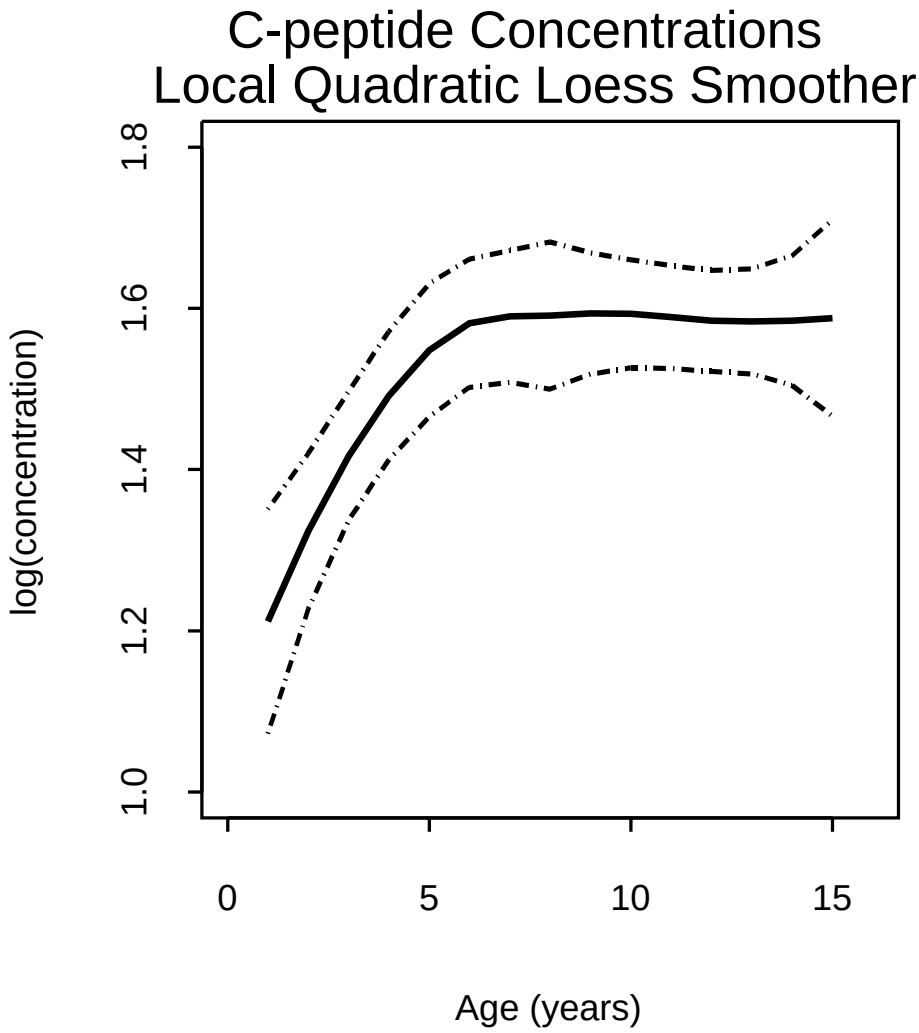

residuals(cpep.lo752)
0.2
0.0
-0.2
1.2
1.3
1.4
1.5
1.6
fitted(cpep.lo752)


residuals(cpep.lo752)
0.2
0.0
-0.2
-2
-1
0
1
2
Quantiles of Standard Normal

```
#  Make predictions using the predict( ) and
#  compute pointwise 95% confidence intervals

cpep.se <- predict(cpep.lo752, seq(1,15,1),
                   se.fit=T)
cpep.locl <- pointwise(cpep.se, coverage=.95)
cpep.locl

$upper:
 [1] 1.350755 1.419861 1.496769 1.570916 1.630554
 [6] 1.661133 1.671951 1.682351 1.668795 1.659994
[11] 1.652856 1.647018 1.648919 1.665167 1.710045

$fit:
 [1] 1.211487 1.323710 1.417012 1.491429 1.547887
 [6] 1.581510 1.590187 1.590938 1.593441 1.593186
[11] 1.589101 1.584477 1.583726 1.584747 1.587834

$lower:
 [1] 1.072218 1.227558 1.337255 1.411942 1.465219
 [6] 1.501887 1.508422 1.499525 1.518086 1.526378
[11] 1.525347 1.521935 1.518533 1.504327 1.465624
```

```
plot(cpep.lo752, confidence=15,coverage=0.95,
          ylim=c(1.0,1.8))


# Plot the curve with approximate pointwise
# confidence limits

par(fin=c(7.0,7.0),pch=18,mkh=.001,mex=1.5,
      plt=c(.2,.8,.2,.8))
plot(cpep$age, cpep$Y, type="n", xlim=c(0,16),
       ylim=c(1.0,1.8), xlab="Age (years)",
       ylab="log(concentration)",
       main="C-peptide Concentrations
\n  Local Quadratic Loess Smoother")
lines(smooth.spline(cpep.locl$x, cpep.locl$fit),
        lty=1,lwd=3)
lines(smooth.spline(cpep.locl$x, cpep.locl$upper ),
        lty=3,lwd=3)
lines(smooth.spline(cpep.locl$x, cpep.locl$lower ),
        lty=3,lwd=3)
```


Y
1.0
1.2
1.4
1.6
1.8
5
10
15
age


C-peptide Concentrations
Local Quadratic Loess Smoother
log(concentration)
1.0
1.2
1.4
1.6
1.8
0
5
10
15
Age (years)