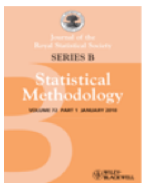
Administration

- HW due February 11 by 1 pm
- Thursday, February 4: TA Li Li has office hours 1-2 (in class), 2-3 in SS 6027A
- Chapter 3: §3.1, 3.2 (except 3.2.4), 3.3 (except 3.3.3), 3.4 (except 3.4.4), 3.5.1
- Chapter 4: §4.1, 4.2, 4.3 (except 4.3.1, 4.3.2), 4.4.0, 4.4.1, 4.4.2
- My office hours are Tuesday 3-4 and Thursday 2-3 (although cancelled on Thursday Feb 4)
- 

  `http://www3.interscience.wiley.com/cgi-bin/fulltext/123233977/HTMLSTART`

  Original Articles

  Sparse partial least squares regression for simultaneous dimension reduction and variable selection (p

  Hyonho Chun, Sündüz Keleş

  Published Online: Jan 6 2010 6:54AM

  DOI: 10.1111/j.1467-9868.2009.00723.x

A few points on logistic regression

- Logistic regression: $Pr(G = k \mid X)$ linear on the logit scale
- Linear discriminant analysis:
  $Pr(G = k \mid X) \propto Pr(X \mid G = k)Pr(G = k)$
- Theory: LDA more efficient if X really is normal
- Practice: LR usually viewed as more robust, but HTF claim prediction errors are very similar
- See: last slide of Jan 26 for calculation of prediction errors on training data
- Data: LR is more complicated with $K > 2$; use `multinom` in the `MASS` library
- Lasso version of logistic regression described in §4.4.4

... logistic regression

- Deviance in a generalized linear model (such as LR), is $-2 \log L(\hat{\beta}) + constant$
- Comparing deviances from two model fits is a log-likelihood ratio test that the corresponding parameters are 0
- AIC compares instead $-2 \log L(\hat{\beta}) + 2p$
- for Binomial data, but not for binary data, residual deviance provides a test of goodness of fit of the binomial model

Flexible modelling using basis expansions

(Chapter 5)

- Linear regression: $y = X\beta + \epsilon, \qquad \epsilon \sim (0, \sigma^2)$
- 'Smooth' regression: $y = f(X) + \epsilon$
- $f(X) = E(Y \mid X)$ to be specified
- Flexible linear modelling

$$f(X) = \Sigma_{m=1}^{M} \beta_m h_m(X)$$

- This is called a linear basis expansion, and h_m is the mth basis function
- For example if X is one-dimensional:
  $f(X) = \beta_0 + \beta_1 X + \beta_2 X^2$, or
  $f(X) = \beta_0 + \beta_1 \sin(X) + \beta_2 \cos(X)$, etc.
- Simple linear regression has $h_1(X) = 1$, $h_2(X) = X$.
  Several other examples on p.140

- Polynomial fits: $h_j(x) = x^j, j = 0, \ldots, m$
- Fit using linear regression with design matrix X, where $X_{ij} = h_j(x_i)$
- Justification is that any 'smooth' function can be approximated by a polynomial expansion (Taylor series)
- Can be difficult to fit numerically, as correlation between columns can be large
- May be useful locally, but less likely to work over the range of X
- Idea: fit polynomials locally in X
- Need to be careful not to overfit, since we are using only a fraction of the data

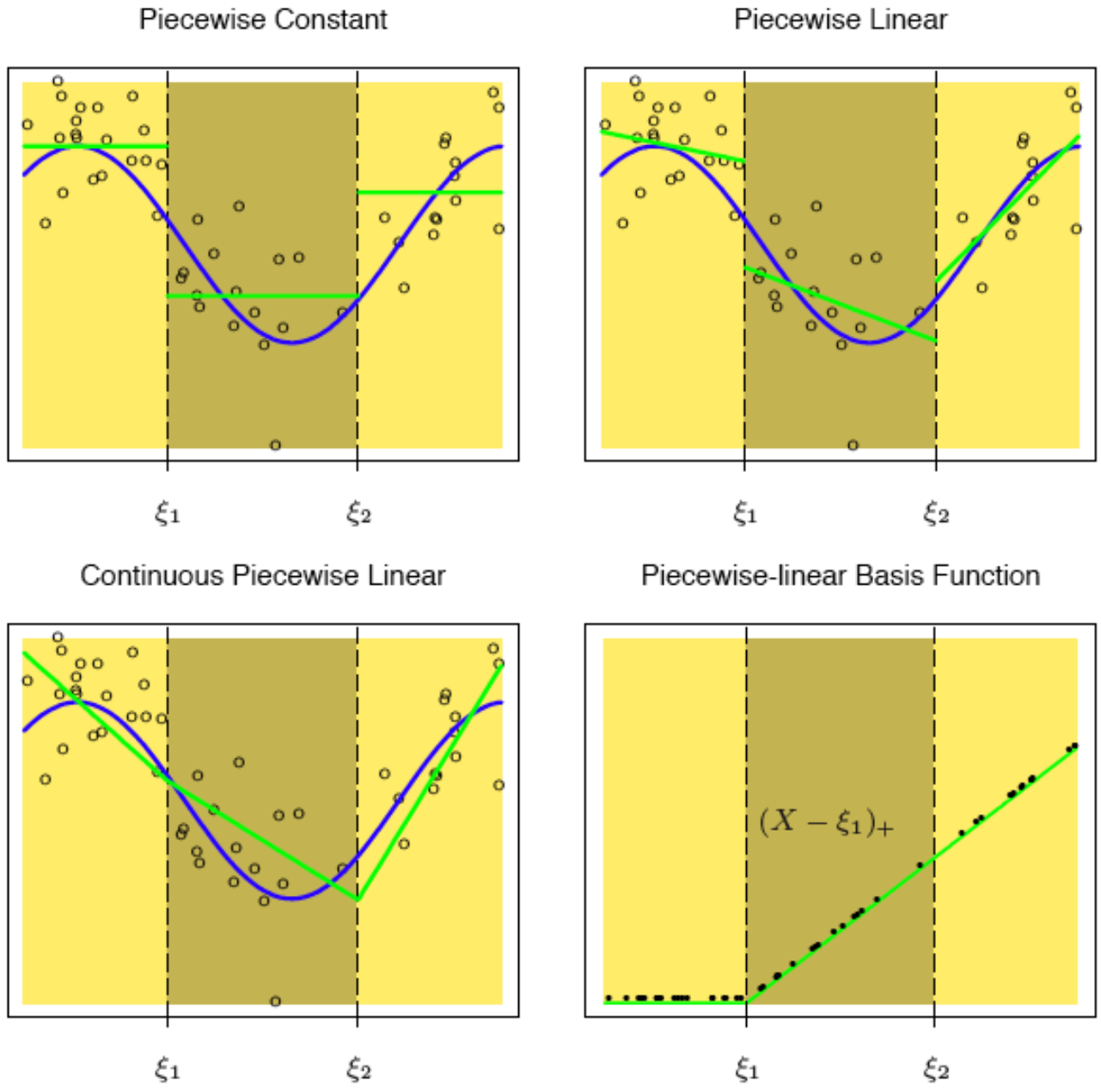
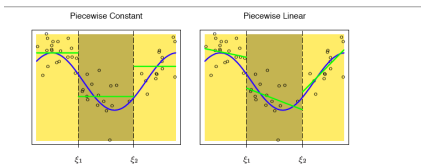


FIGURE 5.1. *The top left panel shows a piecewise constant function fit to some artificial data. The broken vertical lines indicate the positions of the two* knots *ξ_1 and ξ_2. The blue curve represents the true function, from which the data were*

Piecewise polynomials

- piecewise constant basis functions
  $h_1(X) = I(X < \xi_1), \quad h_2(X) = I(\xi_1 \leq X < \xi_2),$
  $h_3(x) = I(\xi_2 \leq X)$
- fitting by local averaging

- piecewise linear basis functions , with constraints
  $h_1(X) = 1, \quad h_2(X) = X$
  $h_3(X) = (X - \xi_1)_+, \quad h_4(X) = (X - \xi_2)_+$
- windows defined by knots $\xi_1, \xi_2, \ldots$



... cubic polynomials

- basis functions
  $h_1(X) = 1, h_2(X) = X, h_3(X) = X^2, h_4(X) = X^3$
- continuity $h_5(X) = (X - \xi_1)^3_+, \quad h_6(X) = (X - \xi_2)^3_+$
- continuous function, continuous first and second derivatives Figure 5.2

Cubic splines

- truncated power basis of degree 3
- need to choose number of knots K and placement of knots $\xi_1, \ldots \xi_K$
- construct features matrix using truncated power basis set
- use constructed matrix as set of predictors

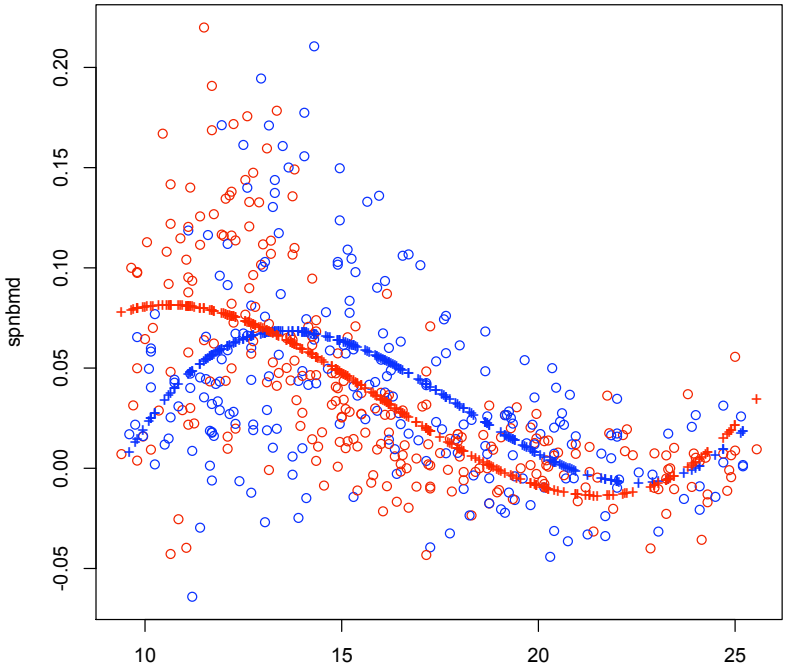
```
> x = 1:10;  cbind(1, x, x^2, x^3); poly(x^3)
> bs(x) ## B-spline basis
                1           2            3
 [1,] 0.00000000 0.00000000 0.000000000
 [2,] 0.26337449 0.03292181 0.001371742
 [3,] 0.40329218 0.11522634 0.010973937
 [4,] 0.44444444 0.22222222 0.037037037
 [5,] 0.41152263 0.32921811 0.087791495
 ...
```

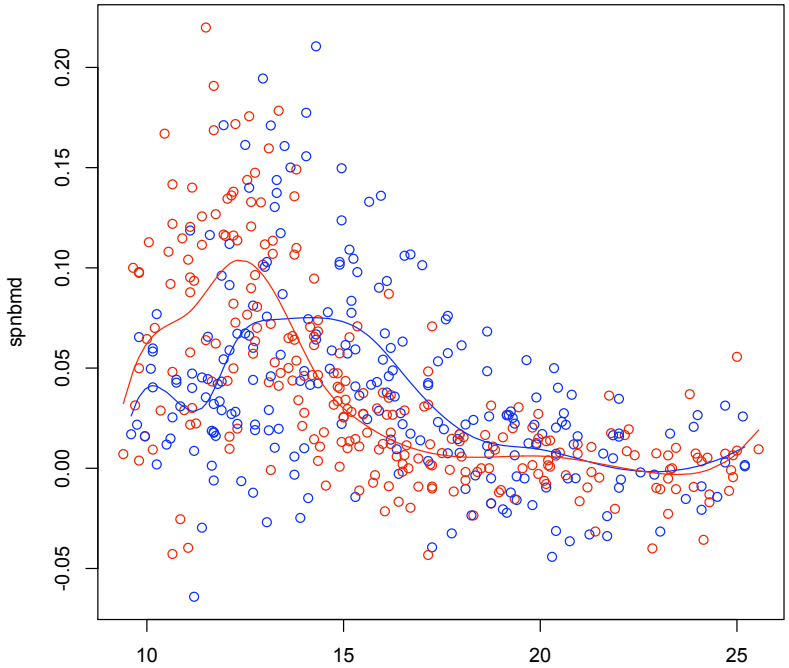
Bone density, Figure 5.6

- `data(bone)` in `ElemStatLearn`
- 485 observations; 226 male, 259, female
- covariate x = age; response y = bone density

... bone density

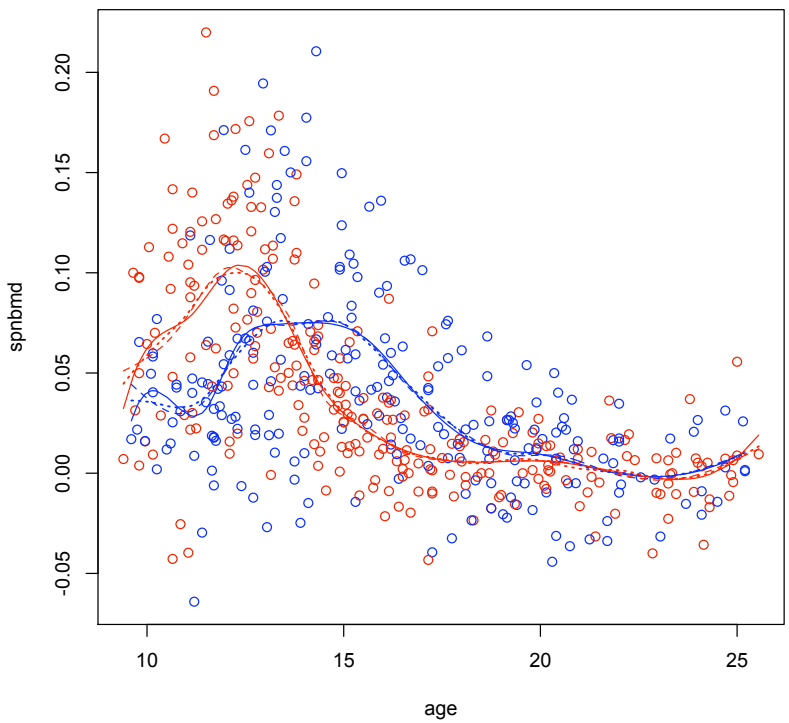
```
> data(bone) # bs(x) with no other arguments just gives a single cubic polynomial
> bone[1:4,]  # bs(x, df=12) gives a proper cubic spline basis, with 9 knots
  idnum   age gender      spnbmd
1     1 11.70   male 0.018080670
2     1 12.70   male 0.060109290
3     1 13.75   male 0.005857545
4     2 13.25   male 0.010263930
...

> bone.bs.m = with(subset(bone,gender=="male"),lm(spnbmd ~ bs(age)))
> bone.bs.f = with(subset(bone,gender=="female"),lm(spnbmd ~ bs(age)))
> plot(spnbmd ~ age, data = bone, col =
+ ifelse(gender=="male", "blue", "red2"))
> points(bone$age[bone$gender=="male"],bone.bs.m$fitted.values,col="blue", pch="+")
> points(bone$age[bone$gender=="female"],bone.bs.f$fitted.values,col="red", pch="+")
```





... useful code

```
> bone.bs.f = with(subset(bone,gender=="female"),lm(spnbmd ~ bs(age,df=12)))
> bone.bs.m = with(subset(bone,gender=="male"),lm(spnbmd ~ bs(age,df=12)))
> ordf = order(bone$age[bone$gender=="female"])
> ordm = order(bone$age[bone$gender=="male"])
> plot(spnbmd ~ age, data = bone, col =
+ ifelse(gender=="male", "blue", "red2"))
> lines(maleage[ordm],bone.bs.m$fitted.values[ordm],col="blue")
> lines(femage[ordf],bone.bs.f$fitted.values[ordf],col="red")
```



Heart data

```
> bs.sbp <- bs(hr$sbp,df=4)     # the B-spline basis
                                # with 4 degrees of freedom
> dim(bs.sbp)
[1] 462   4                   # this is the basis matrix
                              # for the variable "sbp"
> bs.sbp[1:4,]
              1         2          3           4
[1,] 0.16968090 0.4511590 0.34950621 0.029653925
[2,] 0.35240669 0.4758851 0.17002102 0.001687183
[3,] 0.71090498 0.1642420 0.01087580 0.000000000
[4,] 0.09617733 0.3769808 0.44812470 0.078717201
```

Regression splines (p.144) are linear fits to these basis functions

B-splines

- The *B*-spline basis equivalent to the truncated power basis
- Appendix to Ch. 5 describes the construction
- In R `library(splines)`:
  `bs(x, df=NULL, knots=NULL, degree=3, intercept=FALSE, Boundary.knots=range(x))`
- Must specify either `df` or `knots`. For the *B*-spline basis, `# knots = df - degree` and degree is usually 3
- Natural cubic splines are linear at the end of the range (§5.2.1)
- `ns(x, df=NULL, knots=NULL, degree=3, intercept=FALSE, Boundary.knots=range(x))`
- For natural cubic splines, `# knots = df - 1`

... heart data

```
> heart.ns = glm (chd ~ ns(sbp,4)+ ns(tobacco,4) + ns(ldl,4) + famhist + ns(obesity, 4) +
+  ns(age,4), family=binomial)
> summary(heart.ns)

Call:
glm(formula = chd ~ ns(sbp, 4) + ns(tobacco, 4) + ns(ldl, 4) +
    famhist + ns(obesity, 4) + ns(age, 4), family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.7216  -0.8322  -0.3777   0.8870   2.9694

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)     -2.265534   2.367227  -0.957 0.338547
ns(sbp, 4)1     -1.474172   0.843870  -1.747 0.080652 .
ns(sbp, 4)2     -1.351182   0.759548  -1.779 0.075251 .
ns(sbp, 4)3     -3.729348   2.021064  -1.845 0.065003 .
ns(sbp, 4)4      1.381701   0.995268   1.388 0.165055
ns(tobacco, 4)1  0.654109   0.453248   1.443 0.148975
ns(tobacco, 4)2  0.392582   0.892628   0.440 0.660079
ns(tobacco, 4)3  3.335170   1.179656   2.827 0.004695 **
ns(tobacco, 4)4  3.845611   2.386584   1.611 0.107104
ns(ldl, 4)1      1.921215   1.311052   1.465 0.142812
ns(ldl, 4)2      1.783272   1.014883   1.757 0.078897 .
ns(ldl, 4)3      4.623680   2.972938   1.555 0.119885
ns(ldl, 4)4      3.354692   1.447217   2.318 0.020448 *
famhistPresent   1.078507   0.237685   4.538 5.69e-06 ***
ns(obesity, 4)1 -3.089393   1.707207  -1.810 0.070355 .
ns(obesity, 4)2 -2.385045   1.200450  -1.987 0.046945 *
ns(obesity, 4)3 -4.998882   3.796264  -1.317 0.187909
ns(obesity, 4)4  0.009109   1.751127   0.005 0.995850
```

The individual coefficients don't mean anything, we need to evaluate groups of coefficients. We can do this with successive likelihood ratio tests, by hand, e.g.

```
> summary(heart.ns)

 ... stuff omitted
ns(age, 4)3      7.624692   2.560613   2.978 0.002904 **
ns(age, 4)4      1.535277   0.591531   2.595 0.009447 **
---
Signif. codes:  0 Ô***Õ 0.001 Ô**Õ 0.01 Ô*Õ 0.05 Ô.Õ 0.1 Ô Õ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 596.11  on 461  degrees of freedom
Residual deviance: 458.09  on 440  degrees of freedom
AIC: 502.09

Number of Fisher Scoring iterations: 6
```

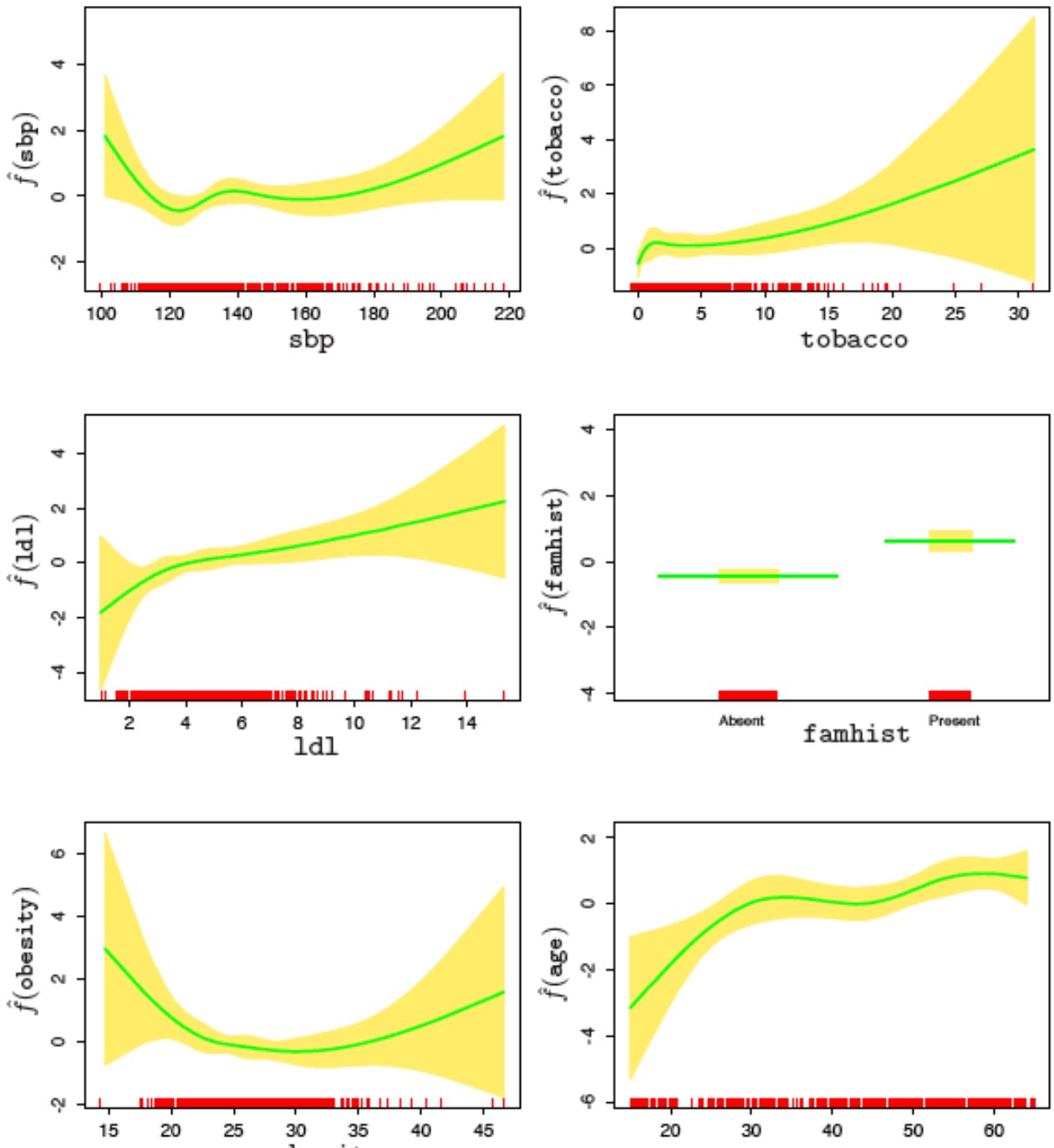
```
> update(heart.ns, . ~ . - ns(sbp,4))

Call:  glm(formula = chd ~ ns(tobacco, 4) + ns(ldl, 4) + famhist + ns(obesity,      4) + ns(a

Coefficients:
    (Intercept)  ns(tobacco, 4)1  ns(tobacco, 4)2  ns(tobacco, 4)3
       -3.91758          0.61696          0.46188          3.51363
ns(tobacco, 4)4      ns(ldl, 4)1      ns(ldl, 4)2      ns(ldl, 4)3
        3.82464          1.70945          1.70659          4.19515
    ns(ldl, 4)4   famhistPresent  ns(obesity, 4)1  ns(obesity, 4)2
        2.90793          0.99053         -2.93143         -2.32793
ns(obesity, 4)3  ns(obesity, 4)4      ns(age, 4)1      ns(age, 4)2
       -4.87074         -0.01103          2.52772          3.12963
    ns(age, 4)3      ns(age, 4)4
        7.34899          1.53433

Degrees of Freedom: 461 Total (i.e. Null);  444 Residual
Null Deviance:     596.1
Residual Deviance: 467.2  AIC: 503.2
> 467.2 - 458.1
[1] 9.1
> pchisq(9.1,df=4)
[1] 0.941352
> 1-.Last.value
[1] 0.05864798  # compare Table 5.1
```

The function `step` does all this for you:

```
> step(heart.ns)
Start:  AIC=502.09
chd ~ ns(sbp, 4) + ns(tobacco, 4) + ns(ldl, 4) + famhist + ns(obesity,
    4) + ns(age, 4)

                Df Deviance    AIC
<none>               458.09 502.09
- ns(obesity, 4)  4   466.24 502.24
- ns(sbp, 4)      4   467.16 503.16
- ns(tobacco, 4)  4   470.48 506.48
- ns(ldl, 4)      4   472.39 508.39
- ns(age, 4)      4   481.86 517.86
- famhist         1   479.44 521.44
 ...
 > anova(heart.ns)
Analysis of Deviance Table

Model: binomial, link: logit

Response: chd

Terms added sequentially (first to last)

               Df Deviance Resid. Df Resid. Dev
NULL                          461     596.11
ns(sbp, 4)      4    19.26       457     576.85
ns(tobacco, 4)  4    46.90       453     529.95
ns(ldl, 4)      4    19.08       449     510.87
famhist         1    25.29       448     485.58
ns(obesity, 4)  4     3.73       444     481.86
ns(age, 4)      4    23.77       440     458.09
```

Notes

- The degrees of freedom fitted are the number of columns in the basis matrix (+ 1 for the intercept).
- This can also be computed as the trace of the hat matrix, which can be extracted from `lm`.
- This works as well for `glm`, because generalized linear models are fitted using iteratively reweighted least squares
- §5.2.3 and §5.3 later
- fitted function $\hat{f}_j(X_j) = h_j(X_j)^T \hat{\theta}_j$ Figure 5.4
- standard errors?


$\hat{f}$(sbp)
sbp
$\hat{f}$(tobacco)
tobacco
$\hat{f}$(ldl)
ldl
$\hat{f}$(famhist)
Absent
Present
famhist
$\hat{f}$(obesity)
$\hat{f}$(age)

Smoothing splines (§5.4)

- ridge regression applied to natural cubic splines
- lots and lots of knots; lead to lots and lots of parameters
- regularize the solution through a penalty term

- New notation: $f(X) = \Sigma_{j=1}^{N} \theta_j N_j(X)$ (5.10)
- knots at each distinct x value
-
$$\min_{\theta} (y - N\theta)^T (y - N\theta) + \lambda \theta^T \Omega_N \theta \quad (5.11)$$
- $N_{ij} = N_j(x_i), \quad \Omega_{jk} = \int N_j''(t) N_k''(t) dt$
- note use of N for set of natural splines
- solution
$$\hat{\theta} = (N^T N + \lambda \Omega_N)^{-1} N^T y$$

Smoothing splines (§5.4)

- solution

$$\hat{\theta} = (N^T N + \lambda \Omega_N)^{-1} N^T y$$

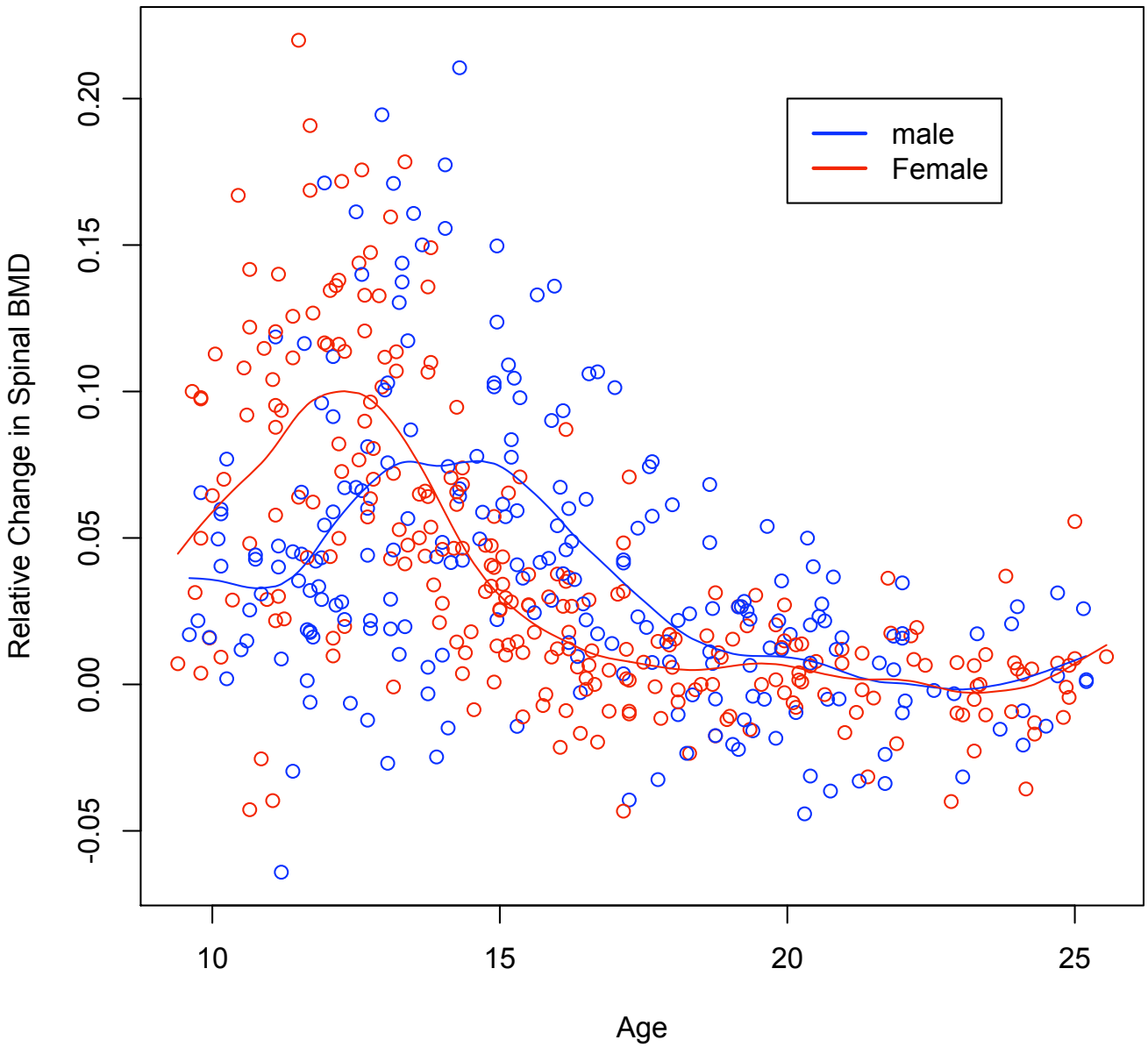
- This solves the variational problem

$$\text{argmin}_f \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda \int_a^b \{f''(t)\}^2 dt$$

- the solution is a natural cubic spline with knots at each x_i
- fitted curve

$$\hat{f}(x) = \sum_{j=1}^{N} N_j(x) \hat{\theta}_j$$

Figure 5.6


male
Female
Relative Change in Spinal BMD
-0.05
0.00
0.05
0.10
0.15
0.20
10
15
20
25
Age

... smoothing splines

- How many parameters have been fit?
- vector of fitted values at the training data

$$\hat{\mathbf{f}} = N(N^T N + \lambda \Omega_N)^{-1} N^T y = S_\lambda y$$

- By analogy with ordinary regression, define the effective degrees of freedom (EDF) as

$$\text{trace } S_\lambda$$

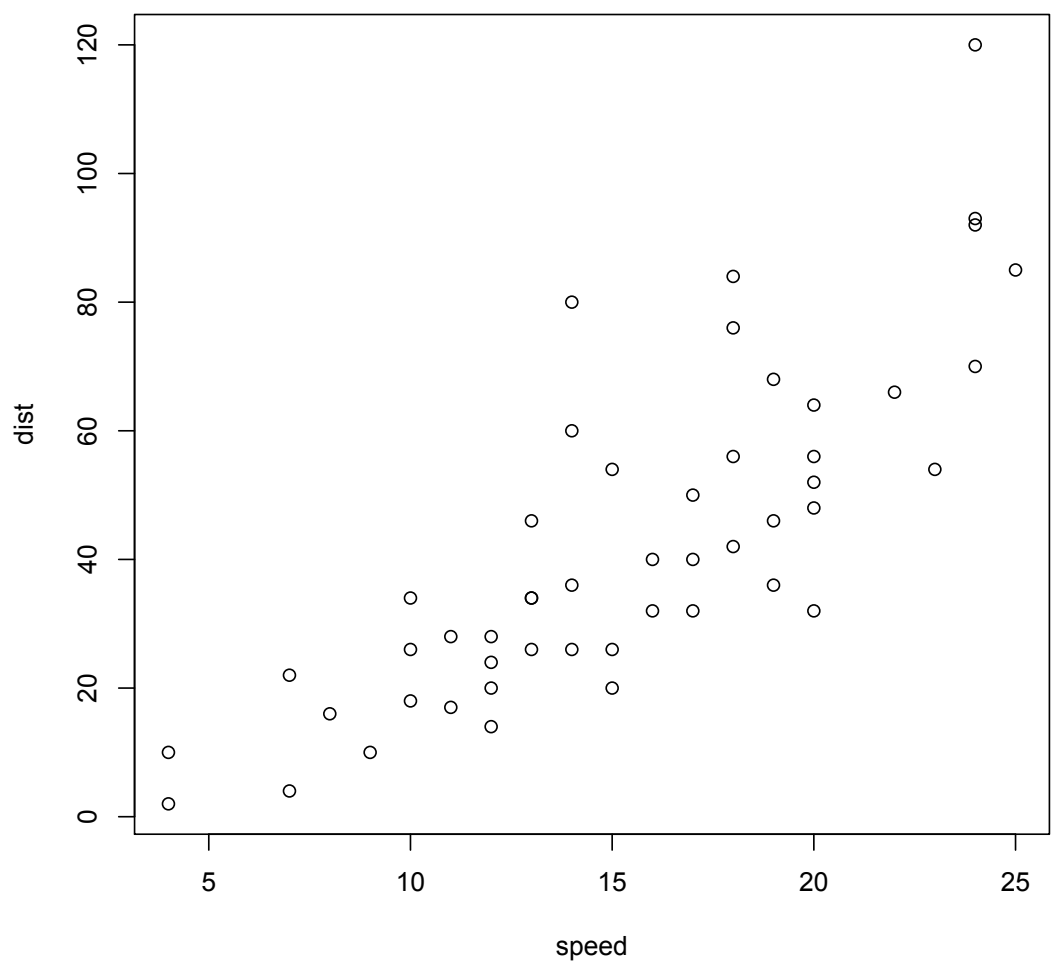
- smoother matrix: symmetric, positive definite
  not a projection matrix
- See p. 153–155 for more details on properties of S_λ
- How to choose λ?
- a) Decide on degrees of freedom to be used, e.g. `smooth.spline(x,y,df=6)`, note that increasing df means less 'bias' and more 'variance'.
- b) Automatic selection by cross-validation (Figure 5.9)

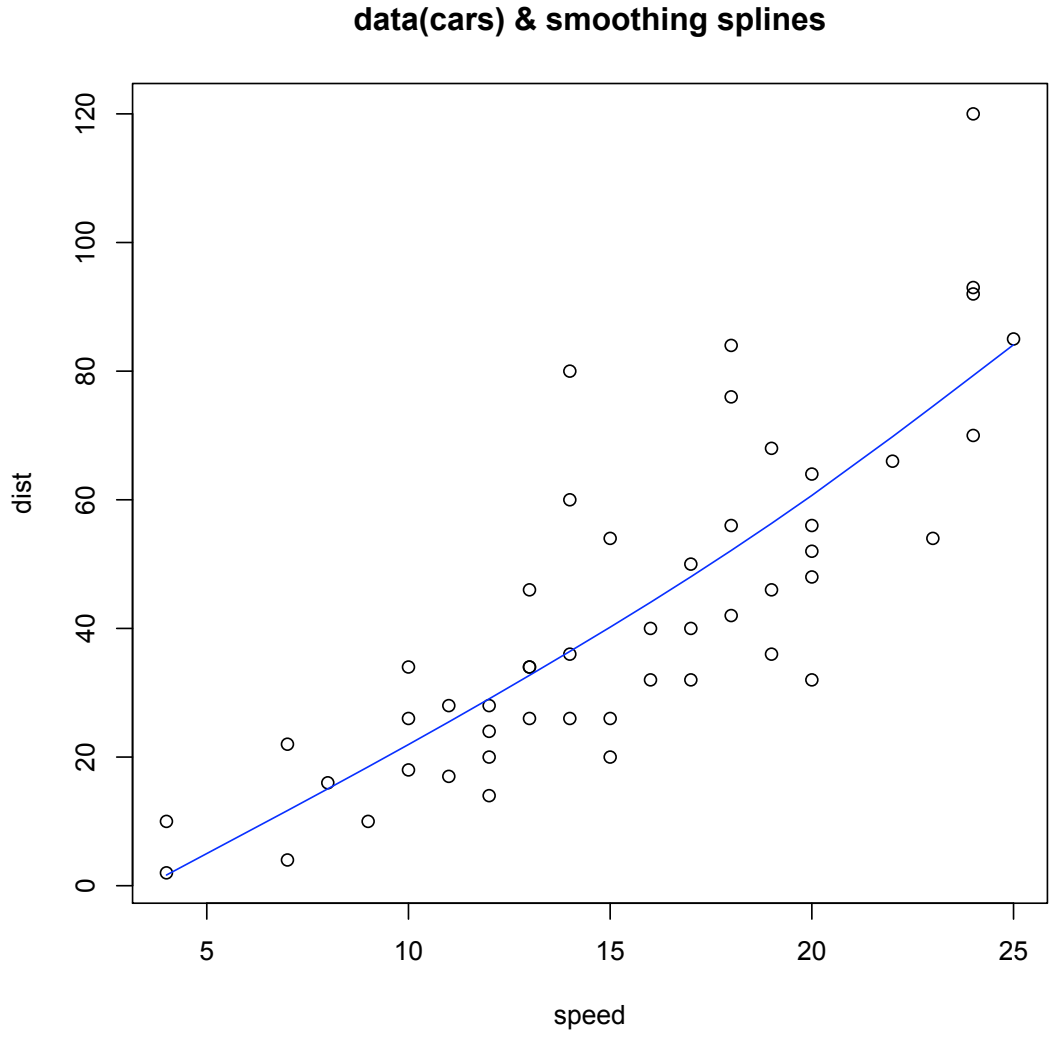
... smoothing splines

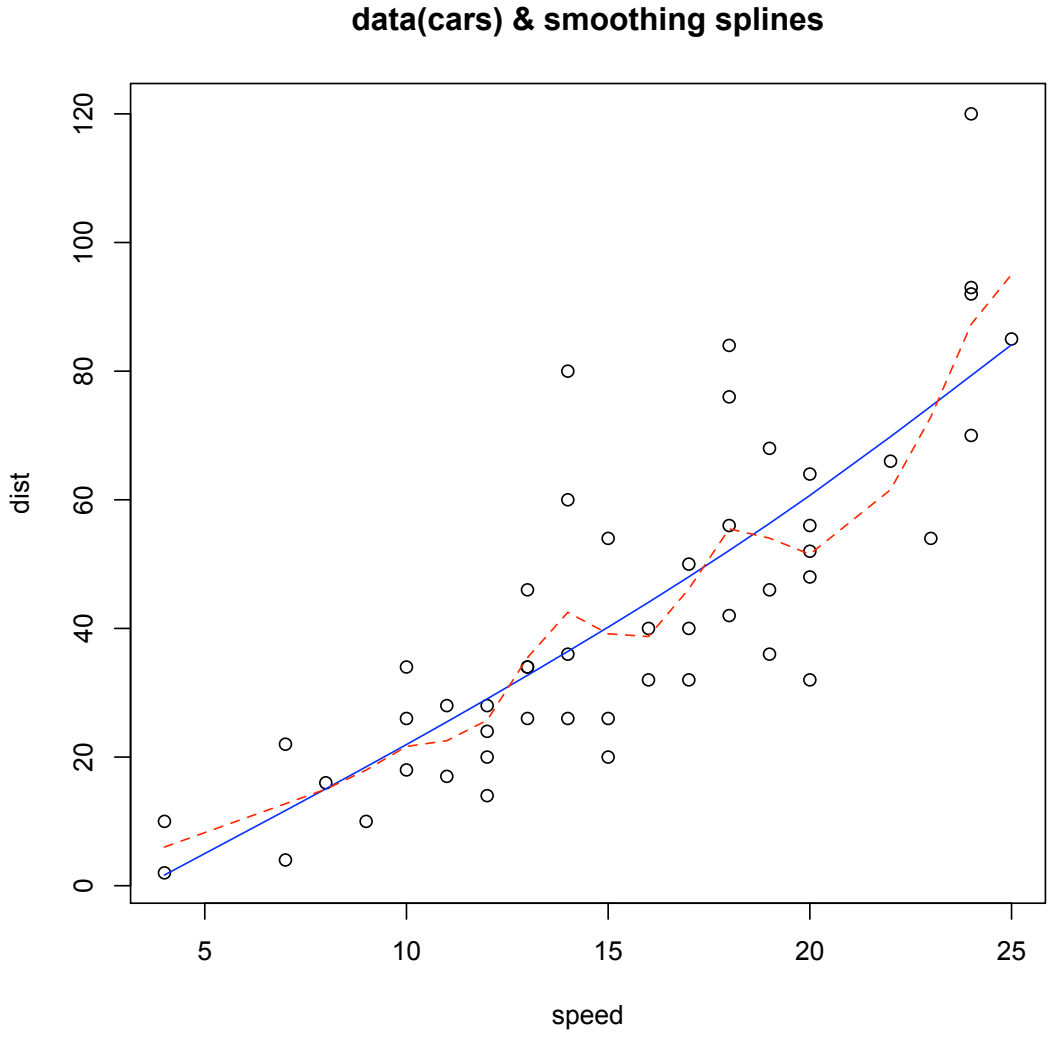
A smoothing spline version of logistic regression is outlined in §5.6, but we'll wait till we discuss generalized additive models.

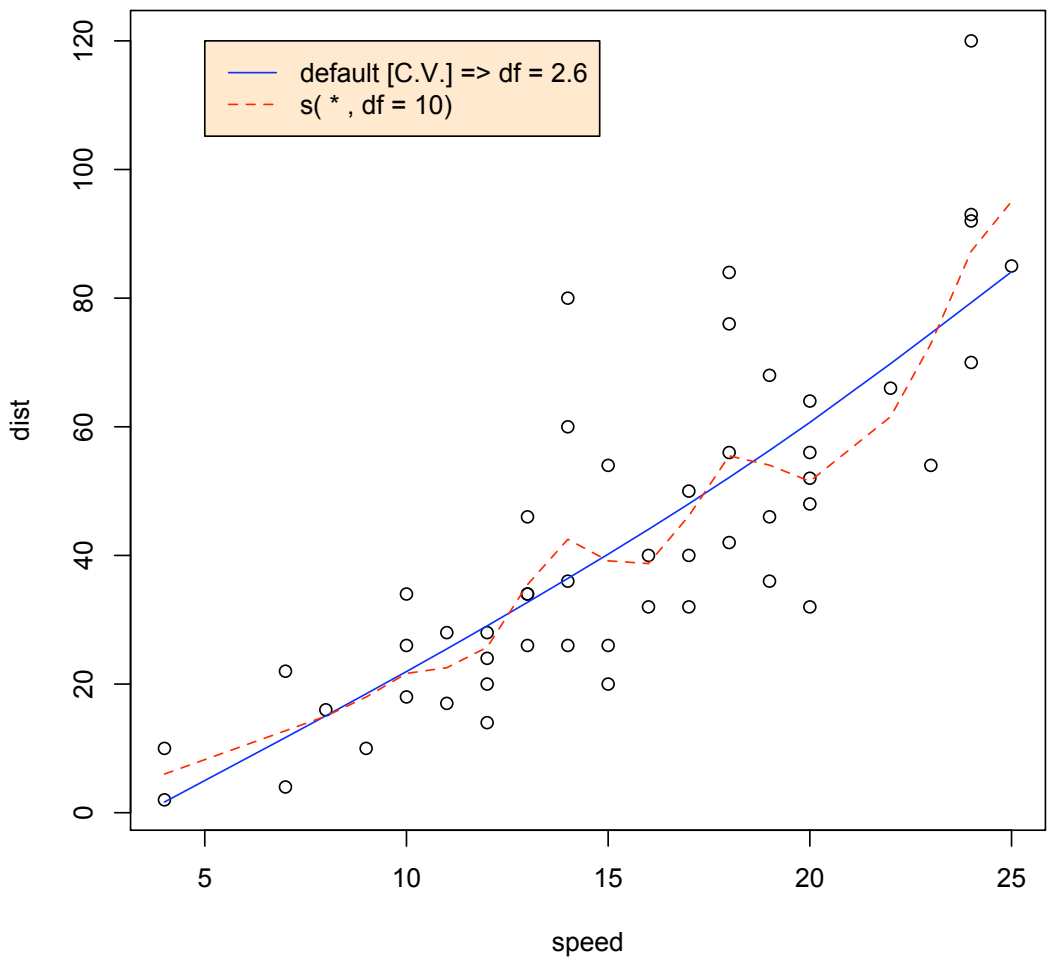
An example from the R help file for `smooth.spline`:

```
> data(cars)
> attach(cars)
> plot(speed, dist, main = "data(cars)  &  smoothing splines")
> cars.spl <- smooth.spline(speed, dist)
> (cars.spl)
Call:
smooth.spline(x = speed, y = dist)

Smoothing Parameter  spar= 0.7801305  lambda= 0.1112206 (11 iterations)
Equivalent Degrees of Freedom (Df): 2.635278
Penalized Criterion: 4337.638
GCV: 244.1044
> lines(cars.spl, col = "blue")
>      lines(smooth.spline(speed, dist, df=10), lty=2, col = "red")
>      legend(5,120,c(paste("default [C.V.] => df =",round(cars.spl$df,1)),
+                     "s( * , df = 10)"), col = c("blue","red"), lty = 1:2,
+             bg='bisque')
> detach()
```


data(cars) & smoothing splines
dist
speed
0
20
40
60
80
100
120
5
10
15
20
25


data(cars) & smoothing splines
dist
speed
0
20
40
60
80
100
120
5
10
15
20
25


data(cars) & smoothing splines
dist
speed
0
20
40
60
80
100
120
5
10
15
20
25


data(cars) & smoothing splines
default [C.V.] => df = 2.6
s(* , df = 10)
dist
speed
0
20
40
60
80
100
120
5
10
15
20
25

Multidimensional splines (§5.7)

- so far we are considering just 1 X at a time
- for regression splines we replace each X by the new columns of the basis matrix
- for smoothing splines we get a univariate regression
- it is possible to construct smoothing splines for two or more inputs simultaneously, but computational difficulty increases rapidly
- these are called thin plate splines
- alternative:
  $E(Y \mid X_1, \ldots, X_p) = f_1(X_1) + f_2(X_2) + \cdots + f_p(X_p)$
  additive models
- binary response:
  $\text{logit}\{E(Y \mid X_1, \ldots, X_p)\} = f_1(X_1) + f_2(X_2) + \cdots + f_p(X_p)$
  generalized additive models