ANALYSIS OF LONGITUDINAL DATA USING CUBIC SMOOTHING SPLINES

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1. Spline smoothing

Suppose that our aim is to model

$$y_i = d(x_i) + \epsilon_i, \ i = 1, \ldots, n,$$

where d is a smooth function and ϵ_i are iid with $E(\epsilon_i) = 0$ and $Var(\epsilon_i) = \sigma_\epsilon^2$.

The linear spline estimator is

$$d(x_i) = \beta_0 + \beta_1 x_i + \sum_{k=1}^{K} u_k (x - \kappa_k)_+,$$

$$(x - \kappa_k)_+ = \begin{cases} 0, & x \le \kappa_k \\ x - \kappa_k, & x > \kappa_k \end{cases}$$

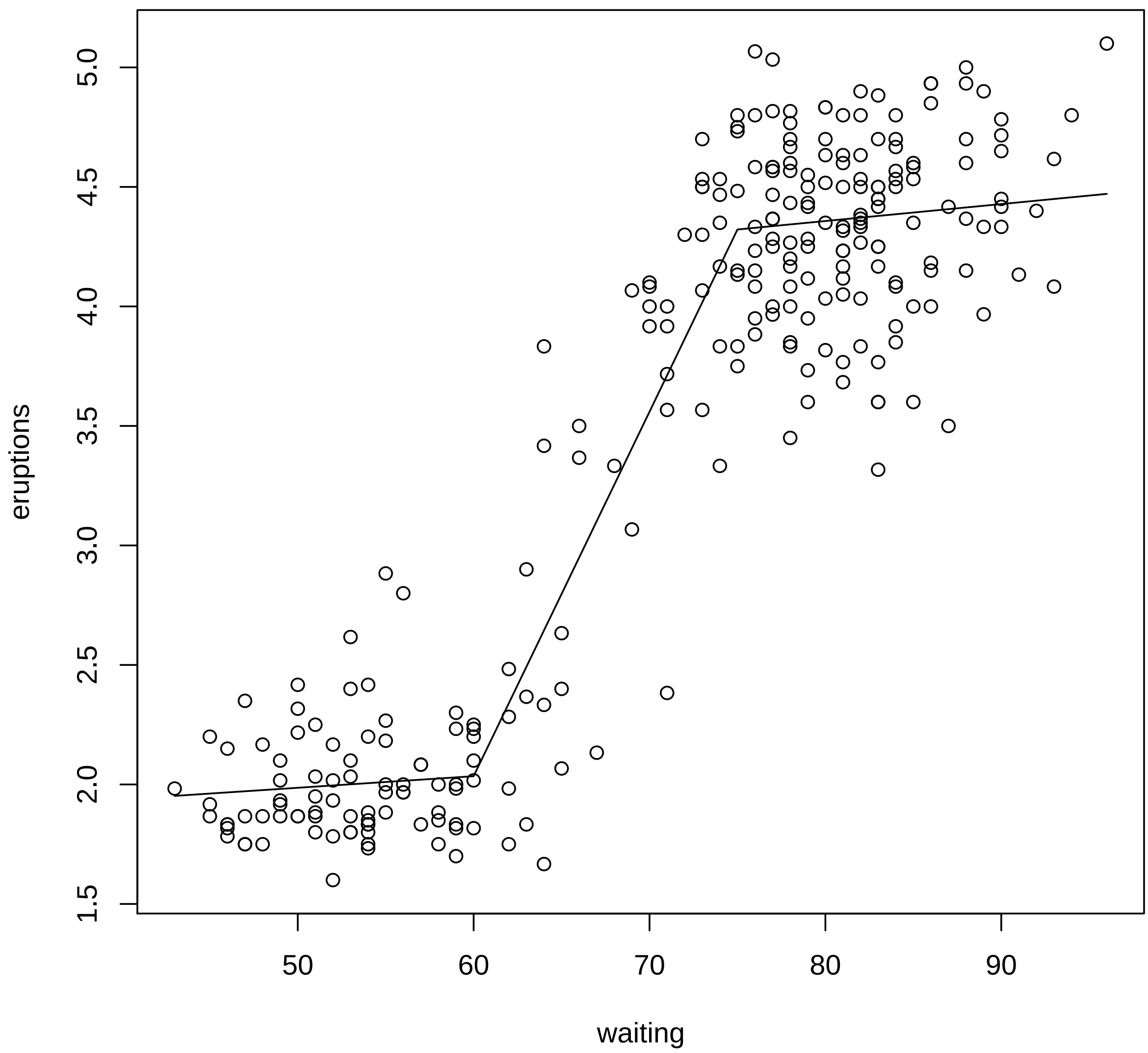
and $\kappa_1, \ldots, \kappa_K$ are $knots$.

The curve d is now modeled by piecewise line segments tied together at knots $\kappa_1, \ldots, \kappa_K$.

Example

```
> library(MASS)
> data(faithful)
> names(faithful)
[1] "eruptions" "waiting"
> plot(faithful)
> faithful<-faithful[order(faithful$waiting),]
> attach(faithful)
> knots<-c(0,60,75) % knots 60, 75
> rhs<-function(x,c) ifelse (x>c,x-c,0)
> dm<-outer(waiting, knots, rhs)
> dm
       [,1] [,2] [,3]
  [1,]   43    0    0
  [2,]   45    0    0
  ...
 [83,]   60    0    0
 [84,]   62    2    0
 ...
[134,]   75   15    0
[135,]   76   16    1
...
```

```
> g<-lm(eruptions~dm)
> plot(eruptions~waiting)
> lines(waiting, predict(g))
>
```



We can generalize the above equation to a piecewise polynomial of degree p, but the most common choices in practice are quadratic ($p = 2$) and cubic ($p = 3$) splines.

For cubic splines we have

$$d(x_i; \boldsymbol{\beta}; \boldsymbol{u}) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \sum_{k=1}^{K} u_k (x - \kappa_k)_+^3,$$

where $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \beta_3)'$, $\boldsymbol{u} = (u_1, \ldots, u_k)'$ and 1, x, x^2, x^3, $(x - \kappa_1)_+^3, \ldots, (x - \kappa_K)_+^3$ are called basis functions. Other possible choices of **basis functions** include B-splines, wavelet, Fourier Series and polynomial bases etc.

A **natural cubic spline** is obtained by assuming that the function is linear beyond the boundary knots.

The number (K) and location of knots $\kappa_1, \ldots, \kappa_K$ must be specified in advance.

Coefficients $\boldsymbol{\beta}$ and $\boldsymbol{u}$ can be estimated using standard least squares procedures.

However, in some cases the estimated curve tends to be a very rough estimate.

Our approach is to apply smoothing splines, where the smoothing is controlled by a smoothing parameter α.

Smoothing splines have a knot at each unique value of x and the fitting is carried out by least squares with a roughness penalty term.

2. Penalized smoothing

If $x_1, \ldots, x_n$ are points in $[a, b]$ satisfying $a < x_1, \ldots, x_n < b$ the penalized sum of squares (PSS) is given as

$$\sum_{i=1}^{n} \{y_i - d(x_i)\}^2 + \alpha \int_a^b \{d''(x)\}^2 dx,$$

where

$$\alpha \int_a^b \{d''(x)\}^2 dx$$

is the roughness penalty (RP) term with $\alpha > 0$.

Note that here α represents the rate of exchange between residual error and local variation.

If α is very large the main component of PSS will be RP and the estimated curve will be very smooth.

If α is relatively small the estimated curve will track the data points very closely.

If we define a non-negative definite matrix

$$\boldsymbol{K} = \boldsymbol{\nabla}\boldsymbol{\Delta}^{-1}\boldsymbol{\nabla}',$$

where non-zero elements of $n \times (n-2)$ matrix $\boldsymbol{\nabla}$ and $(n-2) \times (n-2)$ matrix $\boldsymbol{\Delta}$ are defined as

$$\nabla_{ii} = \frac{1}{h_i},\ \nabla_{i+1,i} = -\left(\frac{1}{h_i} + \frac{1}{h_{i+1}}\right),\ \nabla_{i+2,i} = \frac{1}{h_{i+1}}$$

and

$$G_{i,i+1} = G_{i+1,i} = \frac{h_{i+1}}{6},\ G_{ii} = \frac{h_i + h_{i+1}}{3},$$

where $h_j = x_{j+1} - x_j,\ j = 1, 2, \ldots, n-1$.

Now PSS becomes as

$$PSS(\boldsymbol{K}) = (\boldsymbol{y} - \boldsymbol{d})'(\boldsymbol{y} - \boldsymbol{d}) + \alpha \boldsymbol{d}'\boldsymbol{K}\boldsymbol{d}$$

and its minimum is obtained at

$$\widehat{\boldsymbol{d}} = (\boldsymbol{I} + \alpha \boldsymbol{K})^{-1}\boldsymbol{y}.$$

It can be shown (e.g. Green and Silverman, 1994) that $\widehat{\boldsymbol{d}}$ is a natural cubic smoothing with knots at the points $x_1, \ldots, x_n$.

Note that the special form $\widehat{\boldsymbol{d}}$ follows from the chosen RP term

$$\alpha \int_a^b \{d''(x)\}^2 dx.$$

If we, for example, would use a discrete approximation

$$\mu_{i+1} - 2\mu_i + \mu_{i-1}$$

of the second derivative the PSS would be (Demidenko, 2004)

$$PSS(\boldsymbol{QQ}') = (\boldsymbol{y} - \boldsymbol{d})'(\boldsymbol{y} - \boldsymbol{d}) + \alpha \boldsymbol{d}'\boldsymbol{QQ}'\boldsymbol{d},$$

where ($n = 6$)

$$\boldsymbol{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then the minimizer is

$$\tilde{\boldsymbol{d}} = (\boldsymbol{I} + \alpha \boldsymbol{Q}\boldsymbol{Q}')^{-1}\boldsymbol{y}.$$

Note that for fixed α the spline fit

$$\widehat{\boldsymbol{d}} = (\boldsymbol{I} + \alpha \boldsymbol{K})^{-1}\boldsymbol{y} = \boldsymbol{S}_\alpha \boldsymbol{y}$$

is linear in $\boldsymbol{y}$ and the matrix $\boldsymbol{S}_\alpha$ is known as the *smoother matrix*.

The smoother matrix $\boldsymbol{S}_\alpha$ has many interesting properties discussed e.g. in Hastie, Tibshirami and Friedman (2001), but here I briefly mention only the following :

1. Choosing the smoothing parameter:

$$CV(\alpha) = \sum_{i=1}^{n} \left(\frac{y_i - \widehat{d}_\alpha(x_i)}{1 - S_\alpha(i,i)}\right)^2,$$

   where $S_\alpha(i,i)$ are diagonal elements of $\boldsymbol{S}_\alpha$.

2. Estimation of the effective degrees of freedom

$$df_\alpha = tr(\boldsymbol{S}_\alpha).$$

   This can be compared to matrix

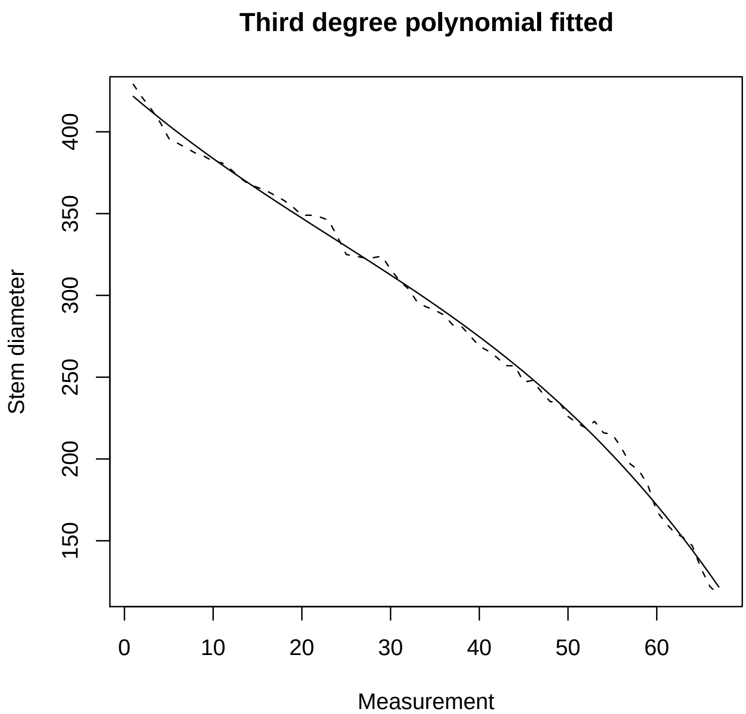
$$\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$$

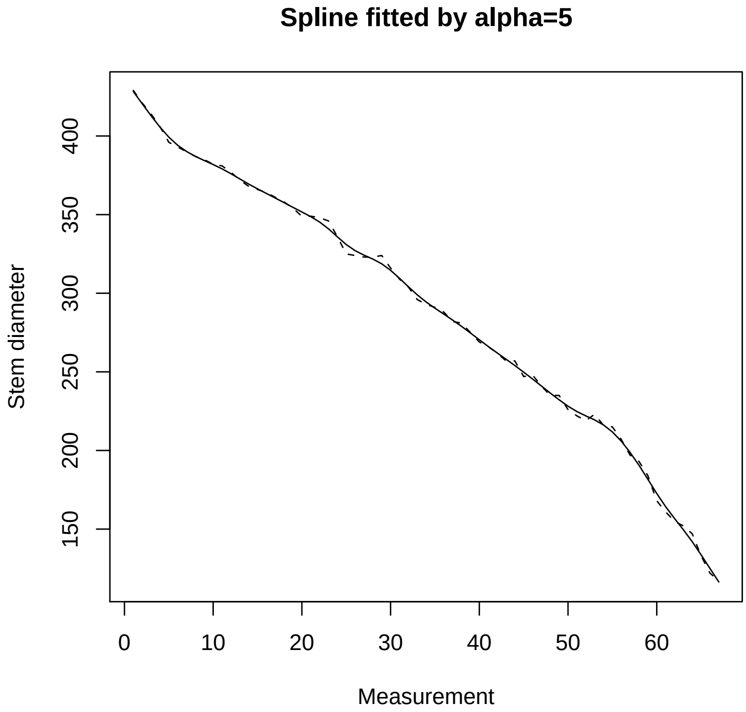
in regression analysis (or in regression splines) in a sense that

$$tr(\boldsymbol{H})$$

gives the number of estimated parameters (or the number of basis functions utilized).

Example: Stem curve model - modelling the degrease of stem diameter as a function stem height.





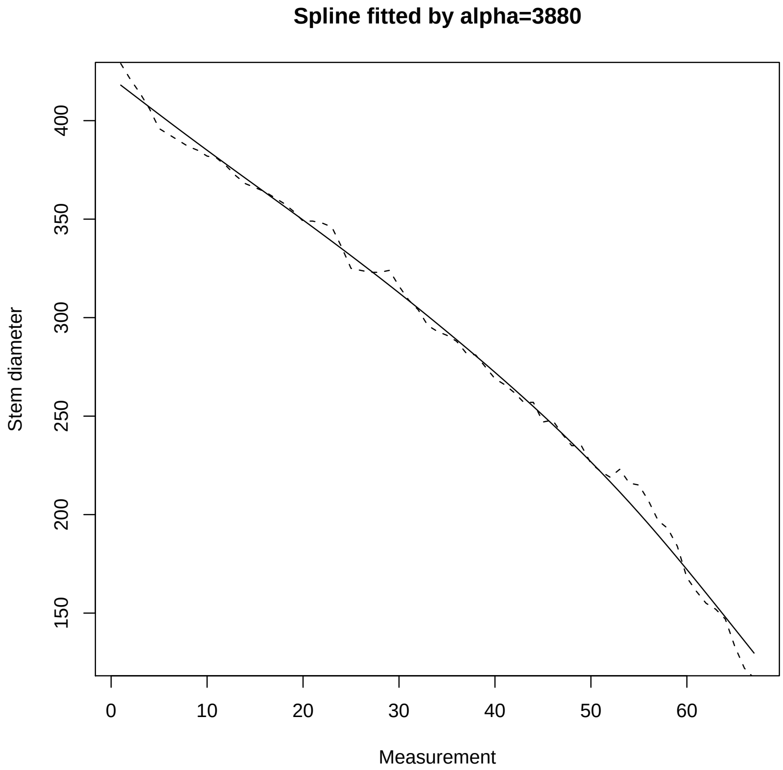
The effective number of degrees of freedom

$df_\alpha = tr(S_{\alpha=5}) = 16.79628.$

Note that if

$$\alpha \to 0,\ \ df_\alpha \to n$$

$$\alpha \to \infty,\ \ df_\alpha \to 2$$



Since $df_\alpha = tr(S_\alpha)$ is monotone in α, we can invert the relationship and specify α by fixing df. For $df = 4$ this gives $\alpha = 3880$.

This yields to model selection with different values for df, where more traditional criteria developed for regression models maybe used.

3. Connection to mixed models

If we let

$$\boldsymbol{X} = [\mathbf{1}, \boldsymbol{x}],$$

where $\boldsymbol{x} = (x_1, \ldots, x_n)'$ and by the special form of $\boldsymbol{\nabla}$ we note that

$$\boldsymbol{X}'\boldsymbol{\nabla} = \mathbf{0}$$

and

$$(\boldsymbol{I}+\alpha\boldsymbol{K})^{-1} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'+\boldsymbol{Z}(\boldsymbol{Z}'\boldsymbol{Z}+\alpha\Delta^{-1})\boldsymbol{Z}',$$

where $\boldsymbol{Z} = \boldsymbol{\nabla}(\boldsymbol{\nabla}'\boldsymbol{\nabla})^{-1}$.

Then the solution of $PSS(\boldsymbol{K})$ can be written as

$$\widehat{\boldsymbol{d}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}} + \boldsymbol{Z}\widehat{\boldsymbol{u}},$$

where

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{y}$$

and

$$\widehat{\boldsymbol{u}} = (\boldsymbol{Z}'\boldsymbol{Z} + \alpha\boldsymbol{\Delta}^{-1})^{-1}\boldsymbol{Z}'\boldsymbol{y}.$$

These estimates can be seen as (BLUP) solutions of the mixed model

$$\boldsymbol{y} = \boldsymbol{X}\beta + \boldsymbol{Z}\boldsymbol{u} + \boldsymbol{\epsilon},$$

where $\boldsymbol{X}$ and $\boldsymbol{Z}$ are defined before and

$$\boldsymbol{u} \sim N(\mathbf{0}, \sigma_u^2\boldsymbol{\Delta}) \text{ and } \boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\boldsymbol{I})$$

with smoothing parameter as a variance ratio $\alpha = \frac{\sigma^2}{\sigma_u^2}$.

Note that we may always rewrite

$$\boldsymbol{y} = \boldsymbol{X}\beta + \boldsymbol{Z}_*\boldsymbol{u}_* + \boldsymbol{\epsilon},$$

where $\boldsymbol{Z}_* = \boldsymbol{Z}\Delta^{1/2}$ and $\boldsymbol{u}_* = \Delta^{-1/2}\boldsymbol{u}$ with

$$\boldsymbol{u}_* \sim N(\boldsymbol{0}, \sigma_u^2\boldsymbol{I}) \text{ and } \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2\boldsymbol{I}).$$

We can now use standard statistical software for parameter estimation (e.g. LME in R or Proc Mixed in SAS).

4. Growth Curves

- The growth curve model (GCM) of Potthoff & Roy (1964)

$$\boldsymbol{Y} = \boldsymbol{T}\boldsymbol{B}\boldsymbol{A}' + \boldsymbol{E},$$

where $\boldsymbol{Y} = (\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_n)$ is a matrix of obs.,
$\boldsymbol{T}$ and $\boldsymbol{A}$ are design matrices (within and between individual),
$\boldsymbol{B}$ is a matrix of unknown parameters, and
$\boldsymbol{E}$ is a matrix of random errors.

- The columns of $\boldsymbol{E}$ are independently distributed as

$$\boldsymbol{e}_i \sim N(\boldsymbol{0}, \boldsymbol{\Sigma}).$$

- Here I assume that

$$\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{R},$$

where $\boldsymbol{R}$ takes certain parsimonious covariance structure with covariance parameters $\boldsymbol{\theta}$.

- Now we may write

$$\boldsymbol{Y} = \boldsymbol{G}\boldsymbol{A}' + \boldsymbol{E},$$

  where $\boldsymbol{G} = (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_m)$ is the matrix of mean curves.

- The GCM is a linear approximation

$$\begin{aligned} \boldsymbol{G} &= (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_m) \\ &= (\boldsymbol{T}\boldsymbol{\beta}_1, \ldots, \boldsymbol{T}\boldsymbol{\beta}_m) \\ &= \boldsymbol{T}\boldsymbol{B}. \end{aligned}$$

- The aim here is to develop the methods needed when $\boldsymbol{G}$ is approximated by more flexible cubic smoothing splines.

- Penalized log-likelihood function

$$2l = -\frac{1}{\sigma^2}\text{tr}[(\boldsymbol{Y}' - \boldsymbol{A}\boldsymbol{G}')\boldsymbol{R}^{-1}(\boldsymbol{Y}' - \boldsymbol{A}\boldsymbol{G}')' +$$

$$\alpha(\boldsymbol{A}\boldsymbol{G}')\boldsymbol{K}(\boldsymbol{A}\boldsymbol{G}')'] - n\log|\sigma^2\boldsymbol{R}| - c.$$

- For given α, σ^2 and $\boldsymbol{R}$, the maximum is obtained at

$$\tilde{\boldsymbol{G}} = (\boldsymbol{R}^{-1} + \alpha\boldsymbol{K})^{-1}\boldsymbol{R}^{-1}\boldsymbol{Y}\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{A})^{-1}.$$

- If $\boldsymbol{R}$ satisfies

$$\boldsymbol{R}\boldsymbol{K} = \boldsymbol{K},$$

this simplifies to

$$\widehat{\boldsymbol{G}} = (\boldsymbol{I} + \alpha\boldsymbol{K})^{-1}\boldsymbol{Y}\boldsymbol{A}(\boldsymbol{A}'\boldsymbol{A})^{-1}.$$

- It is easily seen that

  $\boldsymbol{R} = \boldsymbol{I}$ (Independent),

  $\boldsymbol{R} = \boldsymbol{I} + \sigma_d^2 \mathbf{1}\mathbf{1}'$ (Uniform),

  $\boldsymbol{R} = \boldsymbol{I} + \sigma_{d'}^2 \boldsymbol{X}\boldsymbol{X}'$ (Linear1),

  $\boldsymbol{R} = \boldsymbol{I} + \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}'$ (Linear2)

  satisfies the condition $\boldsymbol{R}\boldsymbol{K} = \boldsymbol{K}$.

- This result can be compared to estimation in linear models, when BLUE coinsides with OLSE.