

Flexible Regression and Smoothing

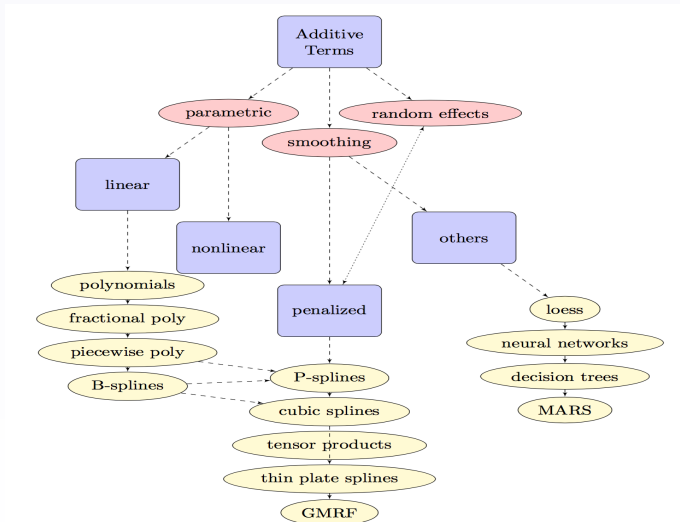
Linear and Smoothing Additive Terms

Mikis Stasinopoulos Bob Rigby

Graz University of Technology, Austria, November 2016

- 1 Introduction
- 2 Linear Additive terms
 - Polynomials
 - Fractional Polynomials
 - Piecewise Polynomials
- 3 Additive Smoothing Terms
 - Local Polynomial Smoothers
 - Penalised Smoothers
 - Types of P-splines smoothers
 - Interface to `gam()`
 - Neural Network
 - Decision Trees

Additive Terms



Additive Terms

model

$$\begin{aligned} \eta = & b_0 + b_1x_1 + b_2x_2 + b_3\text{if}(f = 2) + b_4\text{if}(f = 3) + b_5(x_1 \times x_2) + \\ & b_6x_1\text{if}(f = 2) + b_7x_1\text{if}(f = 3) + s_1(x_3) + s_2(x_4) + \\ & s_3b_8(x_1)x_4 + s_4(x_1)\text{if}(f = 2) + s_5(x_1)\text{if}(f = 3) + s_6(x_3, x_5) \end{aligned}$$

R code

```
m1 <- gamlss(y~x1+x2+f+x1:x2+f:x1+pb(x3)+pb(x4)+
             pvc(x1, by=f)+ga(~s(x3,x5))
```

The CD4 data

Data summary: the CD4 data

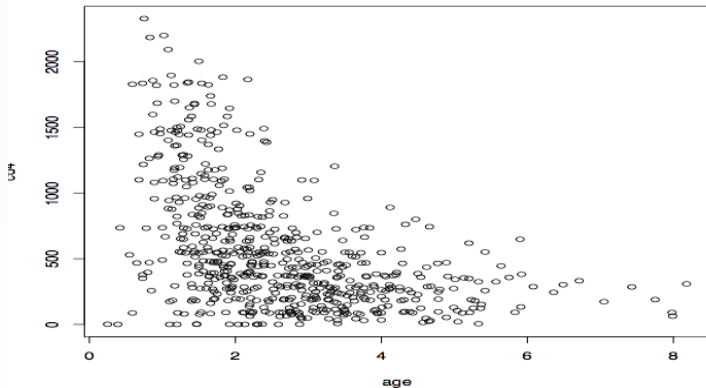
R data file: CD4 in package **MASS** of dimensions 609×2
variables

cd4 : CD4 counts from uninfected children born to HIV-1 mothers.

age : The age of child in in years

purpose: to demonstrate the use of linear parametric terms

The CD4 data: plot



Polynomials

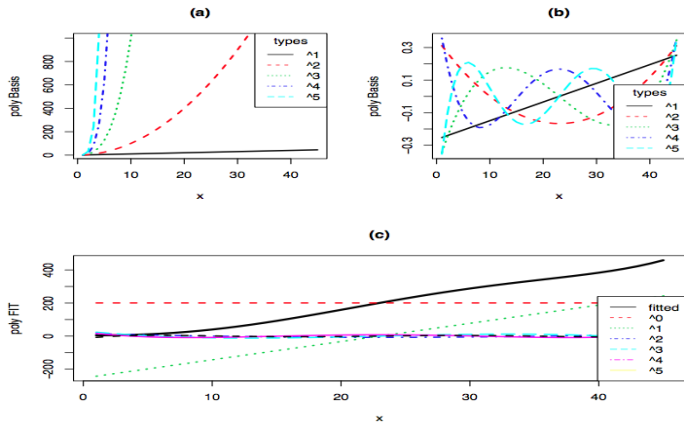
Model

$$h(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \dots + \beta_p x^p$$

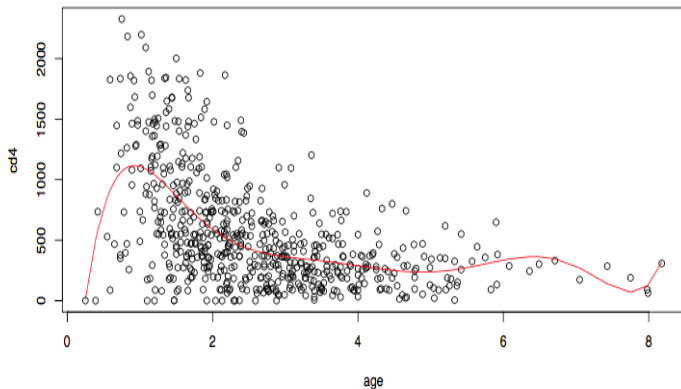
R code

```
m0 <- gamlss(y~x+I(x^2)+I(x^3))  
m1 <- gamlss(y~poly(x,3))
```

Polynomials: basis



CD4 data example, polynomials degree 7



Fractional Polynomials

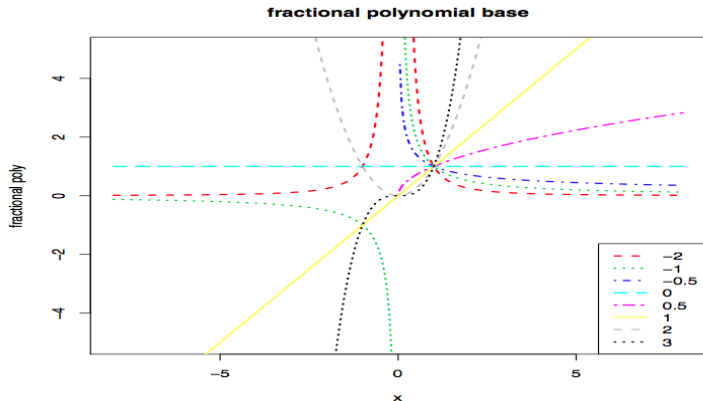
$$\beta_0 + \beta_1 x^{p_1} + \beta_2 x^{p_2} + \beta_3 x^{p_3}$$

where p_j , for $j = 1, 2, 3$ takes values $(-2, -1, -0.5, 0, 0.5, 1, 2, 3)$ with the value 0 interpreted as function $\log(x)$ (rather than x^0).

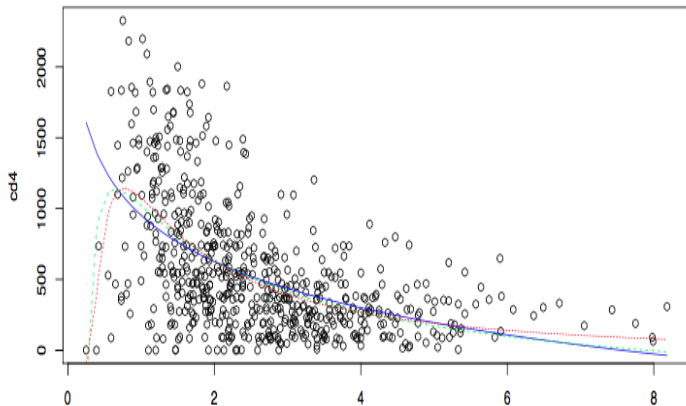
R code

```
m0 <- gamlss(y~fp(x, 3))
```

Fractional Polynomials



CD4 data example, fractional polynomials with 1, 2 and 3 degrees



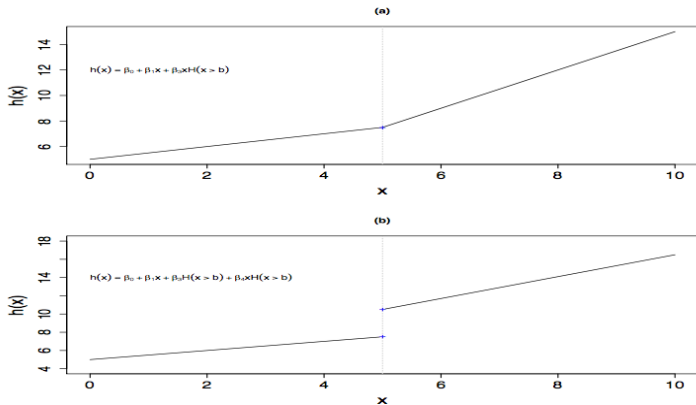
Piecewise Polynomials, Linear + Linear

$$h(x) = \beta_{00} + \beta_{01}x + \beta_{11}(x - b)H(x > b)$$

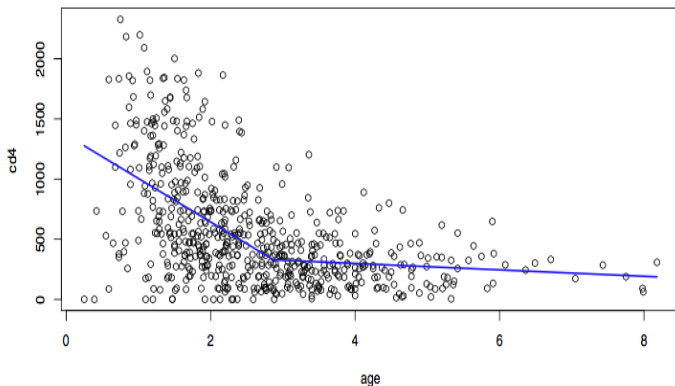
R code

```
f1<-gamlss(cd4~fk(age, degree=1, start=2), data=CD4)
```

Piecewise Polynomials, Linear + Linear



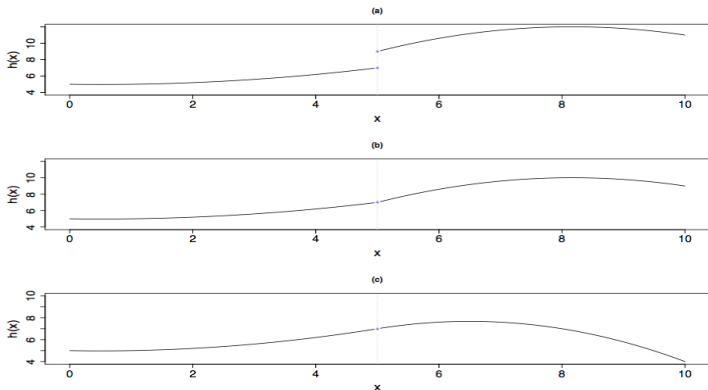
CD4 data example, piecewise polynomials



Piecewise Polynomials, Quadratic + Quadratic

$$h(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + [\beta_{10} + \beta_{11}(x - b) + \beta_{12}(x - b)^2] H(x > b). \quad (1)$$

Piecewise Polynomials, Quadratic + Quadratic



Piecewise Polynomials: splines

$$h(x) = \sum_{j=0}^D \beta_{0j} x^j + \sum_{k=1}^K \sum_{j=0}^D \beta_{kj} (x - b_k)^j H(x > b_k)$$

Splines

$$h(x) = \sum_{j=0}^D \beta_{0j} x^j + \sum_{k=1}^K \beta_k (x - b_k)^D H(x > b_k)$$

cubic splines

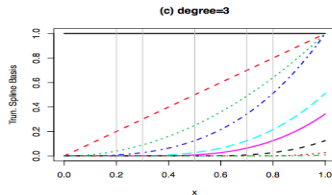
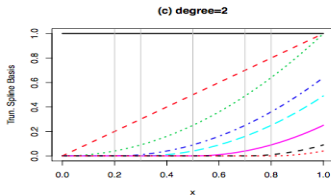
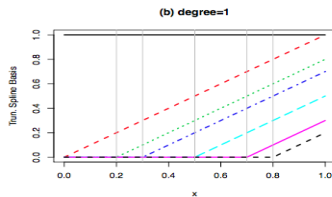
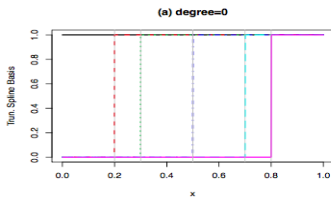
$$h(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{03}x^3 + \sum_{k=1}^K \beta_k (x - b_k)^3 H(x > b_k)$$

natural cubic splines

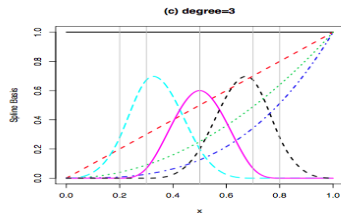
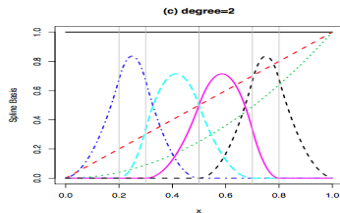
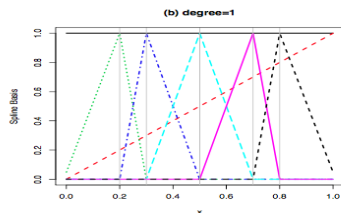
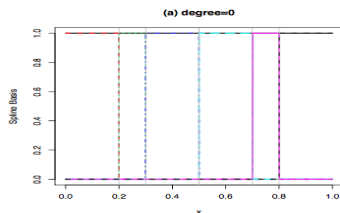
$$h(x) = \beta_{00} + \beta_{01}x + \sum_{k=1}^K \beta_k (x - b_k)^3 H(x > b_k)$$



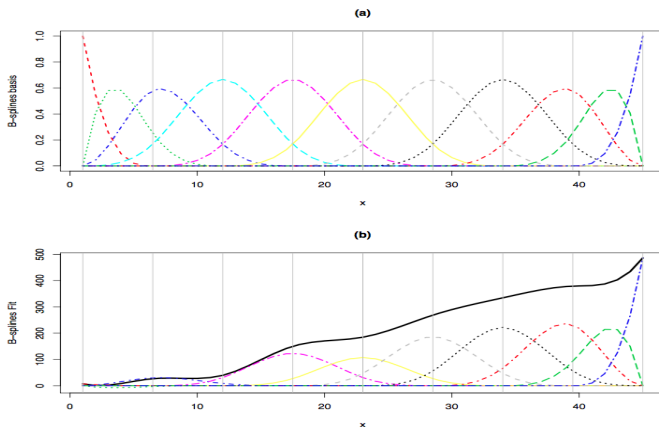
Splines basis: truncated



Splines basis: B-splines



Splines basis, linear function of a B-splines basis

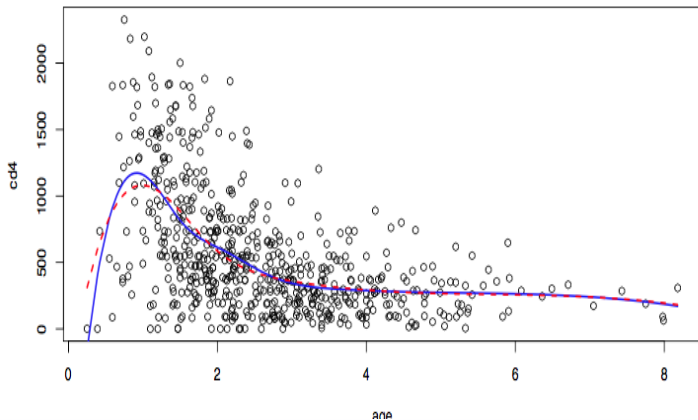


Piecewise polynomial regression

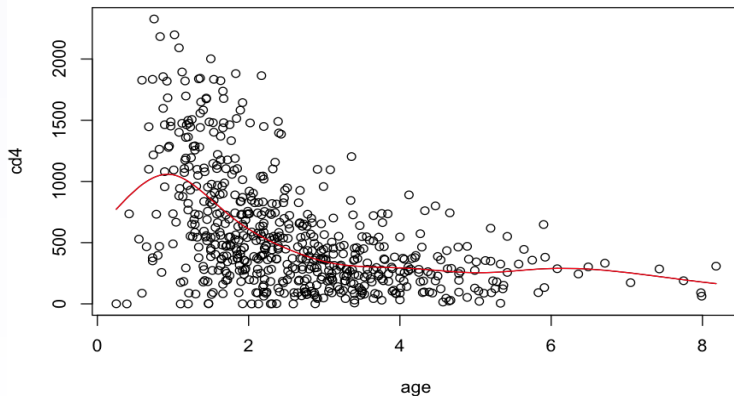
R code

```
m2b <- gamlss(cd4 ~ bs(age), data = CD4)
m3b <- gamlss(cd4 ~ bs(age, df = 3), data = CD4)
m4b <- gamlss(cd4 ~ bs(age, df = 4), data = CD4)
m5b <- gamlss(cd4 ~ bs(age, df = 5), data = CD4)
m6b <- gamlss(cd4 ~ bs(age, df = 6), data = CD4)
m7b <- gamlss(cd4 ~ bs(age, df = 7), data = CD4)
m8b <- gamlss(cd4 ~ bs(age, df = 8), data = CD4)
```

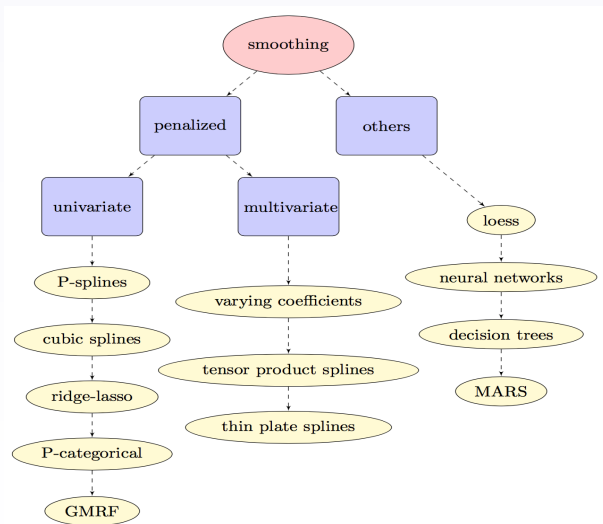
CD4 data example, piecewise polynomials 5, 7 knots



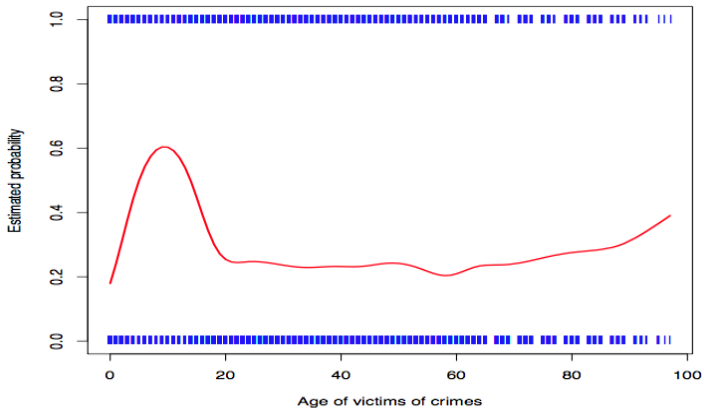
CD4 count data: P-spline fits



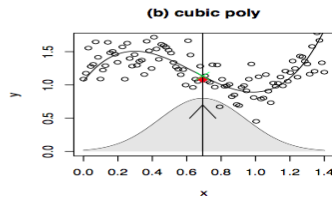
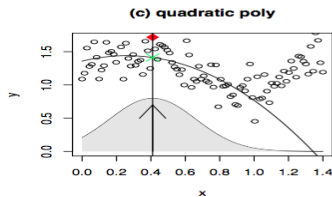
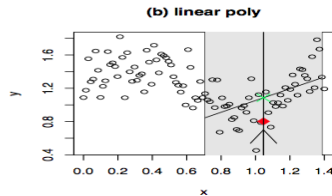
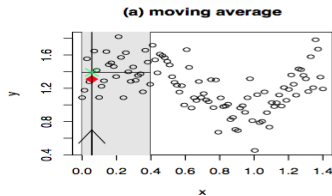
Additive Smoothing Terms: Smoothers



Reported crimes



Local Polynomial Smoothers



Penalised Smoothers

$$Q = (\mathbf{y} - \mathbf{Z}\boldsymbol{\gamma})^\top \mathbf{W}(\mathbf{y} - \mathbf{Z}\boldsymbol{\gamma}) + \lambda \boldsymbol{\gamma}^\top \mathbf{G}\boldsymbol{\gamma}.$$

with solution

$$\hat{\boldsymbol{\gamma}} = \left(\mathbf{Z}^\top \mathbf{W} \mathbf{Z} + \lambda \mathbf{G} \right)^{-1} \mathbf{Z}^\top \mathbf{W} \mathbf{y}.$$

$$\begin{aligned} \hat{\mathbf{y}} &= \mathbf{Z} \left(\mathbf{Z}^\top \mathbf{W} \mathbf{Z} + \lambda \mathbf{G} \right)^{-1} \mathbf{Z}^\top \mathbf{W} \mathbf{y} \\ &= \mathbf{S} \mathbf{y} \end{aligned}$$

Demos

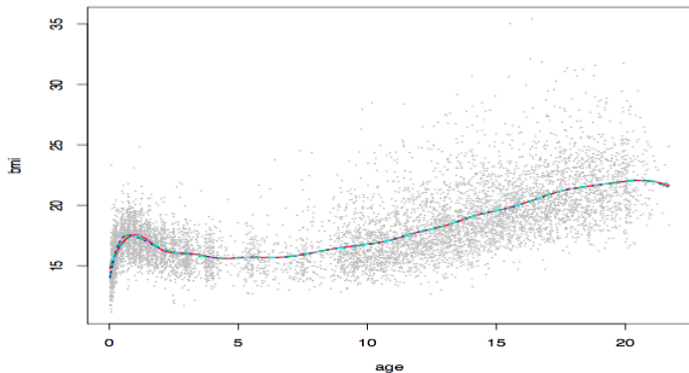
- 1 `demo.BSplines()`
- 2 `demo.RandomWalk()`
- 3 `demo.interpolateSmo()`
- 4 `demo.histSmo()`
- 5 `demo.PSplines()`

P-splines: pb()

R code

```
p1 <- gamlss(bmi~pb(age, method="ML"), data=dbbmi)
p2 <- gamlss(bmi~pb(age, method="GCV") , data=dbbmi)
p3 <- gamlss(bmi~pb(age, method="GAIC", k=2) , data=dbbmi)
p4 <- gamlss(bmi~pb(age, method="GAIC",
                    k=log(length(dbbmi$bmi))),
              data=dbbmi)
```

P-splines: `pb()`

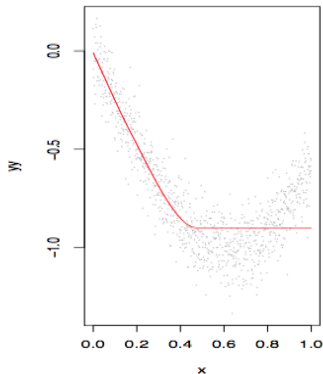
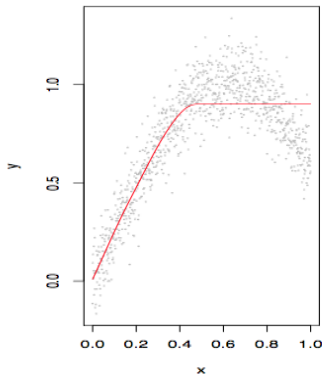


Monotonic P-splines: `pbm()`

R code

```
set.seed(1334)
x = seq(0, 1, length = 1000)
p = 0.4
y = sin(2 * pi * p * x) + rnorm(1000) * 0.1
m1 <- gamlss(y~pbm(x), trace=FALSE)
yy <- -y
m2 <- gamlss(yy~pbm(x, mono="down"), trace=FALSE)
```


Monotonic P-splines

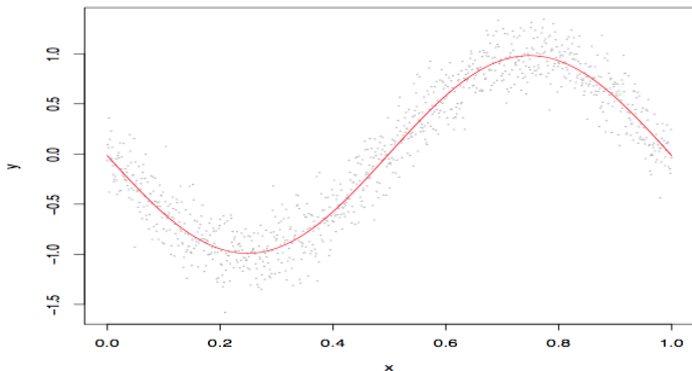


Cycle P-splines: `pb()`, `cy()`

R code

```
set.seed(555)
x = seq(0, 1, length = 1000)
y<-cos(1 * x * 2 * pi + pi / 2)+rnorm(length(x)) * 0.2
m1<-gamlss(y~cy(x), trace=FALSE)
```

Cycle P-splines

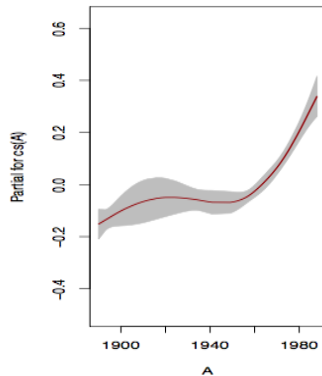
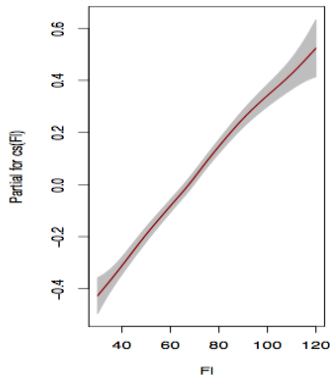


Cubic smoothing splines `cs()`

R code

```
# fitting cubic splines with fixed degrees of freedom  
rcs1<-gamlss(R~cs(Fl)+cs(A), data=rent, family=GA)  
term.plot(rcs1, pages=1)
```

Cubic smoothing splines



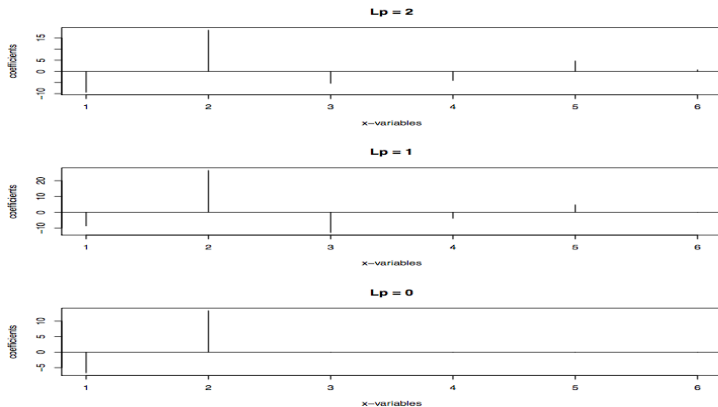
Ridge and Lasso Regression : $ri()$

R code

```
# standardise the data
X<-with(usair, cbind(x1,x2,x3,x4,x5,x6))
sX<-scale(X)
m0<- gamlss(y~sX, data=usair) # least squares
m1<- gamlss(y~ri(sX), data=usair) # ridge
m2<- gamlss(y~ri(sX, Lp=1), data=usair) # lasso
m3<- gamlss(y~ri(sX, Lp=0), data=usair) # best subset
AIC(m0,m1,m2,m3)

##           df           AIC
## m2 5.336309 341.2492
## m0 8.000000 344.7232
## m1 5.884452 345.6097
## m3 2.838310 350.1807
```

Ridge and Lasso Regression

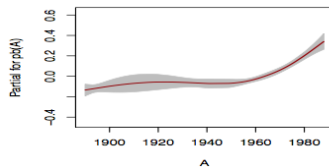
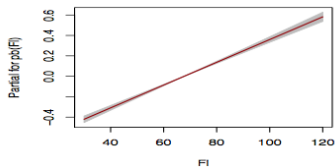


Varying Coefficients Models : `pvc()`

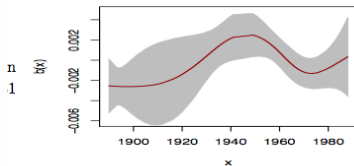
R code

```
m2<-gamlss(R~pb(Fl)+pb(A)+pvc(A, by=Fl), data=rent,  
           family=GA)  
term.plot(m2, pages=1)
```


Varying Coefficients Models



varying coef.

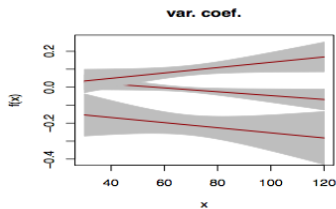
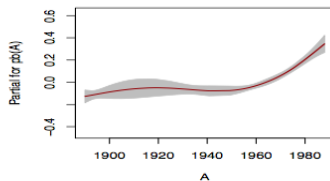
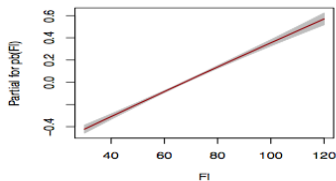


Varying Coefficients Models

R code

```
g1<-gamlss(R~pb(Fl)+pb(A)+pvc(Fl,by=loc), data=rent,  
           family=GA)  
term.plot(g1, pages=1)
```

Varying Coefficients Models

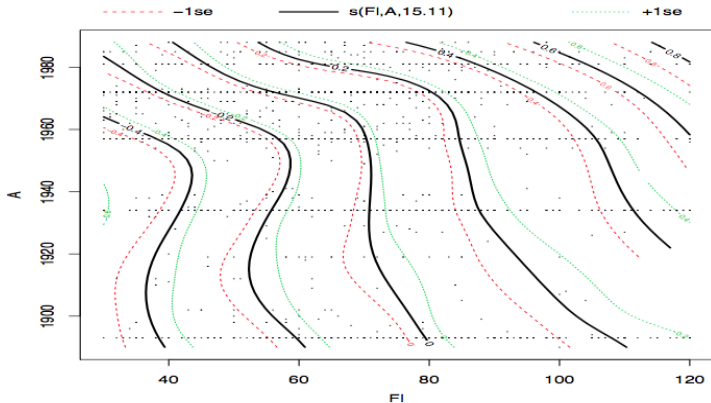


Interface to gam()

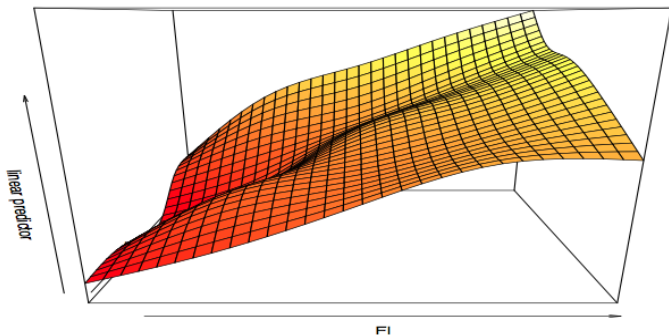
R code

```
ga4 <- gam(R~s(Fl,A), method="REML", data=rent,  
           family=Gamma(log))  
gn4 <- gamlss(R~ga(~s(Fl,A), method="REML"), data=rent,  
             family=GA)  
  
term.plot(gn4)  
vis.gam(getSmo(gn5))
```

Interface to gam()



Interface to gam()

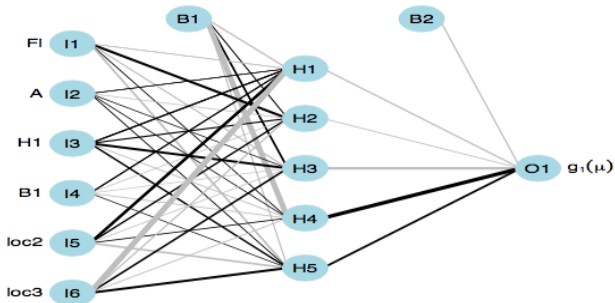


Neural Network: Interface to nnet()

R code

```
mr3 <- gamlss(R~nn(~F1+A+H+B+loc, size=5, decay=0.01),
              data=rent, family=GA)
summary(getSmo(mr3))
## a 6-5-1 network with 41 weights
## options were - linear output units decay=0.01
## b->h1 i1->h1 i2->h1 i3->h1 i4->h1 i5->h1 i6->h1
.....
## -0.13 -0.86 0.05 0.84 0.00 -1.43 2.07
## b->o h1->o h2->o h3->o h4->o h5->o
## -0.28 -0.68 -0.24 -2.39 3.64 1.33
plot(getSmo(mr3), y.lab=expression(g[1](mu)))
```

Interface to nnet()

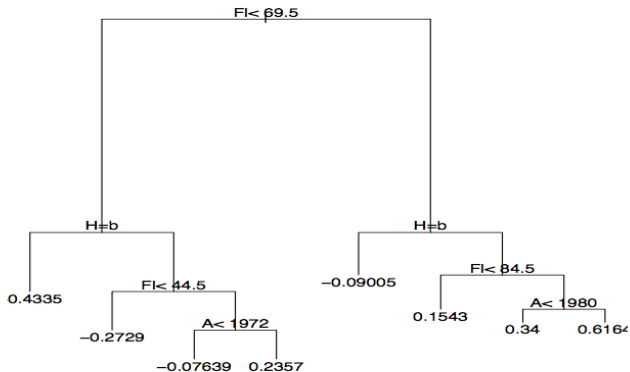


Decision Trees: interface to rpart()

R code

```
r2 <- gamlss(R ~ tr(~Fl+A+H+B+loc),  
              sigma.fo=~tr(~Fl+A+H+B+loc), data=rent,  
              family=GA, gd.tol=100, c.crit=0.1)  
term.plot(r2, parameter="mu", pages=1)
```

Decision Tree interface to rpart()



END

for more information see

www.gamlss.org