Module 5, part II: Penalized and Smoothing Splines

BIOS 526

Reading

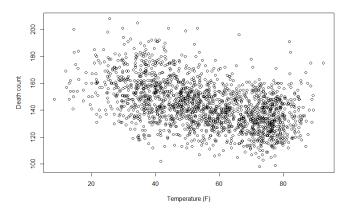
- Sections 5.4 and 5.5 in Hastie et al.
- Sections 3.1 3.14, 4.9 in Ruppert et al.

Concepts

- Constraints and penalized regression.
- Smoothing matrix and smoothing parameter.
- Generalized cross-validation to choose roughness penalty.
- Mixed models to choose roughness penalty.

Motivating Example: Daily Temperature and Deaths

- alldeaths: daily non-accidental deaths in the 5-county New York City, 2001-2005.
- Temp: daily temperature in Fahrenheit.
- > load ("NYC.RData")
- > plot(alldeaths~Temp,xlab="Temperature (F)",ylab ="Death count",data=health)



Regression Problem

Let y_i be the number of non-accidental deaths on day i and x_i be the same-day temperature.

We consider the nonparametric regression problem:

We can approximate $g(x_i)$ using

E.g., linear spline with 9 equidistant interior knots $\kappa_1, \kappa_2, \ldots, \kappa_9$ within the observed range of daily temperature, a piecewise linear spline model is

$$g(x_i) = \beta_0 + \beta_1 x_i + \beta_2 (x_i - \kappa_1)_+ + \beta_3 (x_i - \kappa_2)_+ \dots + \beta_{10} (x_i - \kappa_9)_+$$

Automatic Knot Selection

What if we don't know the number and locations of the knots?

Approach:

- Start with a lot of knots. This ensures that we will not miss important fine-scale behaviour.
- Assume most of the knots are not useful and shrink their coefficients toward zero
- Determine how much to shrink based on some criteria (e.g. GCV or AIC).

Benefits:

- Knot placement is not important if the number is dense enough.
- Shrinking most coefficients to zero will stabilize model estimation similar to performing variable selection.

Penalized Spline

Consider the basis expansion:

Constrain the magnitude of the coefficients β_j .

Consider the ridge-regression penalty:

equivalently,

where $\boldsymbol{\beta}^* = [\beta_2, \dots, \beta_{M+1}]'$ and C is a positive constant.

Penalties

- Ridge regression = |2-penalty = $||\beta^*||_2^2$.
- Other penalties: lasso = absolute value = l1-penalty = $||\beta^*||_1 = \sum_{j=2}^{M+1} |\beta_j|$.
- Ridge shrinks coefficients of vectors in b-spline basis, but does not induce sparsity.
- Ridge is easy to solve closed form solution!
- Lasso tends to make some coefficients exactly zero. Trickier to solve. More on this later in the course.
- A small C will shrink more coefficients, as well as shrink them closer to zero.
- Our goal:

Matrix of g()

For simplicity, consider a linear spline. Then evaluate the basis functions at each x_i , $i=1,\ldots,n$:

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & (x_1 - \kappa_1)_+ & \cdots & (x_1 - \kappa_{M+1})_+ \\ 1 & x_2 & (x_2 - \kappa_1)_+ & \cdots & (x_2 - \kappa_{M+1})_+ \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & (x_n - \kappa_1)_+ & \cdots & (x_n - \kappa_{M+1})_+ \end{bmatrix}$$

Then write $g(x_i)$, i = 1, ..., n in matrix form:

Then the residuals are $\mathbf{Y} - \mathbf{G} = \mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$.

Constrained formulation

We define the objective function:

$$\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \ (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) \ \text{subject to} \ \boldsymbol{\beta}' \mathbf{B} \boldsymbol{\beta} \leq C.$$

Here, ${\bf B}$ is a diagonal matrix with 0 and 1 entries selecting which coefficients are penalized:

Penalized formulation

This problem can be equivalently formulated as

There is a one-to-one mapping between λ and the constraint C. λ is often called the smoothing parameter.

Closed-form solution

$$\underset{\beta}{\operatorname{argmin}} \ (\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta) + \lambda \beta' \mathbf{B}\beta.$$

Differentiate wrt β and set to zero:

$$\begin{aligned} -2\mathbf{X}'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + 2\lambda\mathbf{B}\boldsymbol{\beta} &= 0 \\ -\mathbf{X}'\mathbf{Y} + \mathbf{X}'\mathbf{X}\boldsymbol{\beta} + \lambda\mathbf{B}\boldsymbol{\beta} &= 0 \\ \left(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B}\right)\boldsymbol{\beta} &= \mathbf{X}'\mathbf{Y} \\ \hat{\boldsymbol{\beta}} &= \left(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B}\right)^{-1}\mathbf{X}'\mathbf{Y}. \end{aligned}$$

Closed-form solution

The least squares solution is

for some positive number λ . Note:

- When $\lambda=0$, $\hat{\beta}$ becomes the ordinary least squares estimate. So no penalization is present $(C=\infty)$.
- When $\lambda \to \infty$, $(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1}$ becomes small, so $\hat{\beta}_j \to 0$ if $B_{jj} = 1$.

Mortality and Temperature Example

Consider the death and mortality analysis. Assume 40 equidistant knots and linear splines:

$$y_i = \beta_0 + \beta_1 x_i + \sum_{m=1}^{40} \beta_{1+m} (x_i - \kappa_m)_+$$

We will penalize $\beta_{1+m}, \ldots, \beta_{M+1}$ using the **B** matrix:

Creating piecewise linear spline

We can create a design matrix with piecewise linear splines.

Mortality and Temperature Example

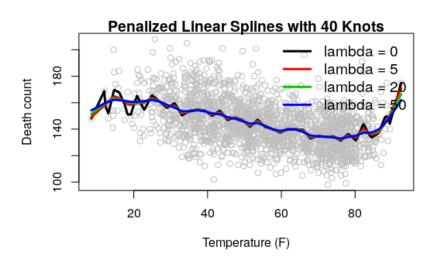
We now search through different values of λ . For each λ , we will

- Calculate the penalized $\hat{\beta}$.
- Calculate $\hat{\boldsymbol{\beta}}' \mathbf{B} \hat{\boldsymbol{\beta}}$.
- Calculate the fitted value $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$.
- Calculate the GCV using the matrix: $\mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1}\mathbf{X}'$.

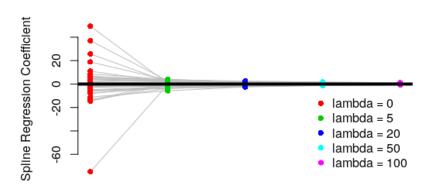
We will select the λ with the smallest GCV.

```
> Y = health$alldeaths
> lambda = 0
> beta = solve (t(X)%*%X + lambda*B) %*% t(X) %*% Y
> H = X %*% solve (t(X)%*%X + lambda*B) %*% t(X) ##Hat matrix
> Yhat = X%*%beta ##Fitted values
> GCV = mean ( (Y-Yhat)^2 ) / (1- mean (diag(H)))^2
> C = t(beta)%*%B%*%beta
```

Effects of Penalization



Effects of Penalization: Shrinkage



Shrinkage

General principle:

- \uparrow shrinkage \rightarrow variance.
- \uparrow shrinkage \rightarrow bias.

How do we determine the tuning parameter λ ?

In other words, how do we determine how much we should shrink?

Effective Degrees of Freedom

With the constraint $\beta' \mathbf{B} \beta < C$, $\hat{\beta}$ is no longer the ordinary least squares estimate.

Let $\hat{\mathbf{Y}} = \mathbf{SY}$ where \mathbf{S} is a smoothing matrix.

In ridge regression, $\mathbf{S} = \mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1}\mathbf{X}'$.

Each element is shrunk towards zero. We can define an effective degrees of freedom df_{eff} as

Note:

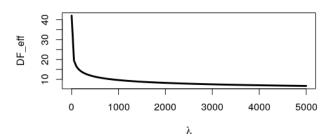
Hence, "effective" df.

Effective Degrees of Freedom, cont.

Note when $\lambda=0$, $df_{\lambda}=rank(\mathbf{X})=p$, the degrees of freedom without penalization.

As $\lambda \uparrow$,

Effective DF



Generalized Cross-validation Error, revisited

We previously defined GCV:

Note that $\hat{\mathbf{Y}} = \mathbf{HY}$ where $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$.

Now we can apply GCV to any prediction of ${\bf Y}$ that can be written in the form:

$$\hat{\mathbf{Y}} = \mathbf{SY}.$$

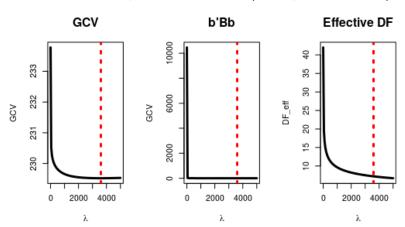
Then GCV is defined:

$$\mathsf{GCV} =$$

This is the definition we will use hereafter.

Smoothing Parameter Selection

Penalized linear splines with 40 knots. (GCV-optimal $\lambda = 3600$)



Residual Error Variance Estimate

Recall our model is

$$y_i = g(x_i) + \epsilon_i \qquad \epsilon_i \stackrel{iid}{\sim} N(0, \sigma^2) .$$

We now have an estimate $\hat{g}(x_i)$. How about σ^2 ?

We have two options:

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n [y_i - \hat{g}(x_i)]^2}{n - df_{\text{eff}}}.$$
 (6)

The above is a biased estimate. Some software gives you the option to use

$$\hat{\sigma}_{\text{unbiased}}^2 = \frac{\sum_{i=1}^n [y_i - \hat{g}(x_i)]^2}{n - 2\text{tr}\{\mathbf{S}\} + \text{tr}\{\mathbf{SS}'\}} \,. \tag{7}$$

Variance of $\hat{g}(x_i)$

Now we can calculate uncertainty associated with $\hat{g}(x_i)$ at each x_i .

With slight abuse of notation, let x_i' be the row vector of basis function values for x_i .

The variance of $\hat{g}(x_i)$ is

Note: you should decide whether or not to include the variance due to the intercept. If $x_i[1] = 1$, then the variance estimate of $\hat{g}(x_i)$ includes this source of uncertainty.

Confidence interval and prediction interval

Obtain point-wise confidence interval derived from previous expression by plugging in $\hat{\sigma}^2$ for σ^2 .

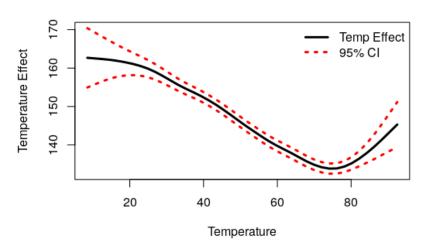
If
$$\lambda = 0$$
:

Similarly the variance for an unobserved point y_i^* with covariate x_i^* has variance

$$Var[\,y_i^*\,] = \sigma^2 + \sigma^2 {\boldsymbol{x}_i^*}'(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1}(\mathbf{X}'\mathbf{X})(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1} \boldsymbol{x}_i^* \;.$$

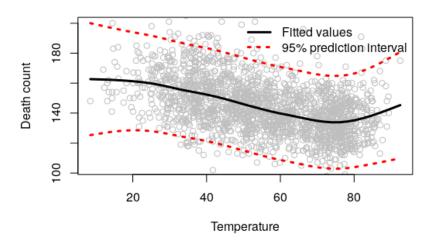
Temperature Effect on Mortality: pointwise CI

```
> Upper95.ci = Yhat + 1.96* sqrt(diag (pred.vcov))
> Lower95.ci = Yhat - 1.96* sqrt(diag (pred.vcov))
```



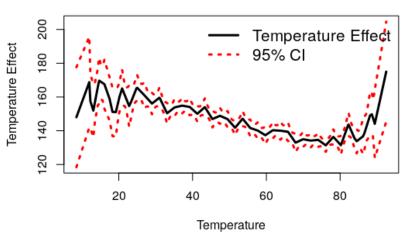
Daily Mortality Prediction

```
> Upper95 = Yhat + 1.96* (sigma1 + sqrt(diag (pred.vcov)) )
> Lower95 = Yhat - 1.96* (sigma1 + sqrt (diag (pred.vcov)) )
```



Temperature Effect on Mortality

Compare to a model without penalization ($\lambda = 0$).



Smoothing Splines: other penalties

A function with large second derivatives can be interpreted as rougher, as the function is allowed to change very rapidly.

We now add a "roughness" penalty to encourage smoothness:

Smoothing spline, cont.

$$\hat{g}(x) = \operatorname*{arg\,min}_{g \in \mathcal{G}} \ \{\mathbf{Y} - g(\tilde{\boldsymbol{x}})\}' \{\mathbf{Y} - g(\tilde{\boldsymbol{x}})\} + \lambda \int \{g''(x;\boldsymbol{\beta})\}^2 \, dx.$$

where \mathcal{G} is the class of twice-differentiable functions and $\tilde{x} \in \mathbb{R}^n$ is the vector of x_i , i = 1, ..., n.

- Note that first derivatives are not penalized.
- The second part uses the squared second-derivative that is a good measure of roughness.
- Shrinks coefficients in a cubic polynomial, causing function to change less quickly.
- λ determines the relative importance of minimizing the residual sum of squares or the roughness.

Smoothing Spline

It turns out the solution $\hat{g}(x)$ is a "natural cubic spline" (a cubic spline with linearity at the boundaries) with knots at the observed points x_i .

More generally, the objective function in (8) with penalized second derivatives is equivalent to

for a certain **B** matrix based on second moments of the basis functions, no longer diagonal; see Ruppert et al p. 75.

The key point is that (9) is a general formula applying to different ridge-like penalties for certain **B**.

As before,

- for a given λ , we can estimate g(x) using penalized least squares;
- search through λ to minimize GCV or another criterion.

Package mgcv in R

The mgcv (Mixed GAM Computation Vehicle) package in R contains the gam() function to fit a large variety of smoothing splines with automatic smoothing parameter selection. We will examine different options throughout the class.

Default option is given in parenthesis.

- Basis functions (default: thin plate regression spline).
- Basis dimension (default: k=10 with one constraint: $\sum \hat{g}(x_i)=0$, makes max edf=9).
- Selection methods (default: GCV).
- Family (default: Gaussian).
- Standard error computation (default: Bayesian).

Temperature Effect on Mortality

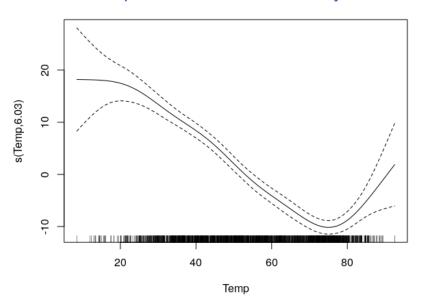
```
> library (mgcv)
> fit1 = gam(alldeaths~s(Temp), data= health)
> summarv(fit1)
Family: gaussian
Link function: identity
Parametric coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 143.917 0.354 407 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Approximate significance of smooth terms:
        edf Ref.df F p-value
s(Temp) 6.03 7.2 80.6 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' '1
R-sq.(adj) = 0.241 Deviance explained = 24.3\%
GCV = 229.47 Scale est. = 228.58 n = 1826
```

mgcv::gam output

```
Approximate significance of smooth terms:
    edf Ref.df F p-value
s(Temp) 6.03 7.2 80.6 <2e-16 ***
---
Signif. codes: 0 '*** 0.001 '** 0.05 '.' 0.1 ' ' 1
R-sq.(adj) = 0.241 Deviance explained = 24.3%
GCV = 229.47 Scale est. = 228.58 n = 1826
```

- edf = effective Df for $tr(\mathbf{S})$.
- Ref edf = effective Df for $2tr(\mathbf{S}) tr(\mathbf{S'S})$.
- Scale est. = estimated residual error σ^2 (using edf).
- F statistic: approximate significance of Temp. Uses Ref edf.
- Use plots to interpret $\hat{g}(x_i)$.

Temperature Effect on Mortality



Checking gam

The default is k=10, such that highest possible EDF is 9 (because of identifiability constraint).

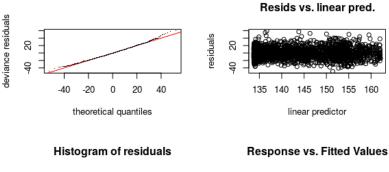
```
> gam.check(fit1)
```

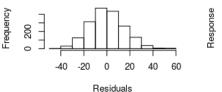
Method: GCV Optimizer: magic Smoothing parameter selection converged after 5 iterations. The RMS GCV score gradient at convergence was 7.242e-05. The Hessian was positive definite. Model rank = 10 / 10

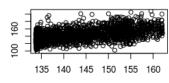
Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

k' edf k-index p-value s(Temp) 9.00 6.03 1.02 0.88

gam.check plots



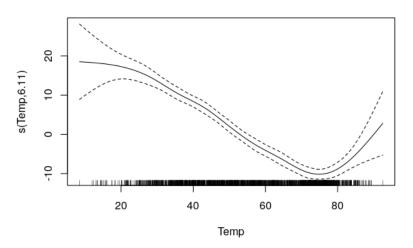




Fitted Values

Temperature Effect on Mortality using cubic

> fit.checkcubic = gam(alldeaths~s(Temp,bs='cr',k=10),method='GCV.Cp',data=health)



Temperature Effect on Mortality

Thin plate splines with k = 40.

```
> fit2= gam (alldeaths s(Temp, k = 40), data = health)
> summary (fit2)
Formula:
alldeaths \sim s(Temp, k = 40)
Parametric coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 143.917 0.354 407 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' '1
Approximate significance of smooth terms:
        edf Ref.df F p-value
s(Temp) 6.23 7.85 73.9 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
R-sq.(adj) = 0.241 Deviance explained = 24.3%
GCV = 229.51 Scale est. = 228.6 n = 1826
```

Extract Useful Model Statistics

Full list see ?gamObject.

• AIC (with edf at penalized estimates)

```
> AIC (fit)
[1] 15109.62
```

Variance-covariance matrix

```
> dim (fit$Ve) ### Frequentist's
[1] 10 10
> dim (fit$Vp) ### Bayesian
[1] 10 10
```

- Fitted value
 - > fit\$fitted

Penalized splines as BLUPs

- GCV may undersmooth.
- An alternative is to treat the coefficients of the truncated polynomials as random effects, and then use BLUPs.
- For concreteness, consider a linear spline:

$$y_i = \beta_0 + \beta_1 x_i + \sum_{m=1}^{M} \theta_m (x_i - \kappa_m)_+ + \epsilon_i,$$
$$\theta_m \stackrel{iid}{\sim} N(0, \tau^2), \quad \epsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$$

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \ \boldsymbol{\Theta} = \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_M \end{bmatrix} \ \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \ \mathbf{Z} = \begin{bmatrix} (x_1 - \kappa_1)_+ & \dots & (x_1 - \kappa_M)_+ \\ \vdots & & \vdots \\ (x_n - \kappa_1)_+ & \dots & (x_n - \kappa_M)_+ \end{bmatrix}$$

Mixed model for estimating a penalized spline

Given τ^2 and σ^2 , we seek to minimize

$$\frac{1}{\sigma^2}||\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\Theta}||^2 + \frac{1}{\tau^2}||\boldsymbol{\Theta}||_2^2,$$

which we can think of ridge regression with penalty $\lambda = \frac{\sigma^2}{\tau^2}$.

We estimate all parameters from the data using the mixed modeling tools we previously learned, and thus obtain a model-based estimate of λ .

Selecting penalty using mixed models

- In mgcv::gam, we can use the option method='REML'
- · Often results in greater smoothing

```
> fit.reml = gam(alldeaths~s(Temp,bs='tp',k=10),method="REML", data= health)
> summary(fit.reml)
Family: gaussian
Link function: identity
Formula:
alldeaths ~ s(Temp, bs = "tp", k = 10)
Parametric coefficients:
          Estimate Std. Error t value Pr(>|t|)
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' 1
Approximate significance of smooth terms:
        edf Ref.df F p-value
s(Temp) 5.499 6.665 86.66 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
R-sq.(adi) = 0.24 Deviance explained = 24.3%
-REML = 7555.7 Scale est. = 228.66 n = 1826
```

Estimate the slope at a particular x_i

```
In linear regression \hat{y}_i=\hat{\beta}_0+\hat{\beta}_1x_i.
In GAMs, we have \hat{y}_i=\hat{\beta}_0+\hat{g}(x_i), and slope changes with x_i. What is the rate of change at 40 degrees Fahrenheit?
```

```
> # visually check whether this is consistent with the plot
> newd <- health[1, ] # grab any row; we are going to change temperature only
> newd$Temp <- 40 - 1e-05 # subtract some small number
> y1 <- predict(fit.reml, newd)
> newd$Temp <- 40 + 1e-05 # add some small number
> y2 <- predict(fit.reml, newd)
> (y2 - y1)/2e-05
49
-0.525
```

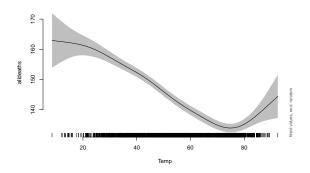
Interpretation

We interpret smoothers $\hat{g}(x_i)$ by looking at plots.

We can add some details regarding the slopes at particular x_i .

Deaths are highest at cold temperatures (<10 degrees F) and slightly decreasing until approximately 20 degrees. Then deaths decrease at a similar rate from approximately 25 to 75 degrees. The number of deaths decreases by approximately 0.5 people / degree in a neighborhood of 40 degrees. Then the number of deaths starts to increase around 75 degrees. At 85 degrees, the number of deaths increases by approximately 0.8 for every 1 degree increase in temperature.

g(x) Interpretation



Additive model with random intercept

Recall the Nepal arm circumference dataset.

Data on 200 children collected at a maximum of 5 time points about 4 months apart.

Consider a non-linear effect of age and a random intercept:

Additive model with random intercept

```
fit.gamm = gam(arm's(age)+s(id,bs = 're'),method='REML',data=nepal)
> gam.check(fit.gamm)

Method: REML Optimizer: outer newton
full convergence after 6 iterations.
Gradient range [-4.190947e-07,-8.779523e-09]
(score 894.436 & scale 0.236499).

Hessian positive definite, eigenvalue range [1.077516,461.7172].

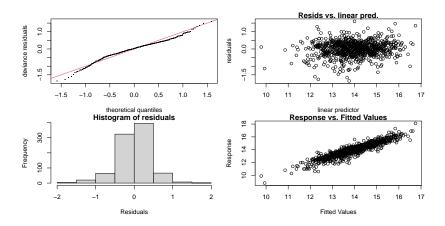
Model rank = 207 / 207

Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

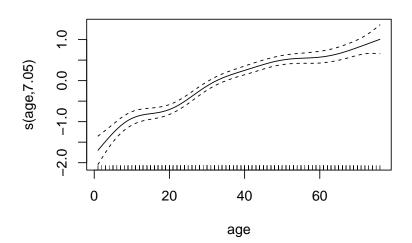
k' edf k-index p-value
s(age) 9.00 7.05 1.03 0.79
s(id) 197.00 181.43 MA NA
```

- I tend to prefer REML
- EDF somewhat close to k'. Other diagnostics okay.
- R code looks at k=20 and results are similar (edf=8.5), so either this model or the one with k=20 is fine.
- For random effect, k' equals number of subjects. Good to check this because will try to fit a smooth if you don't code as a factor.

Additive mixed model with random intercept



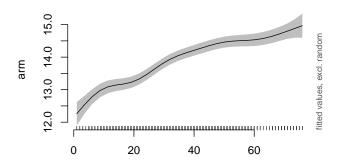
Effect of age on arm circumference



Effect of age on arm circumfenerece

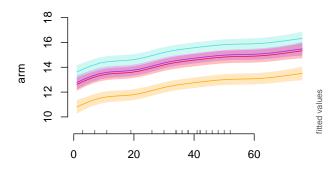
This plot includes the intercept:

- > library(itsadug)
- > plot_smooth(fit.gamm,view='age',rm.ranef=TRUE)
 Summary:
- * age : numeric predictor; with 30 values ranging from 1.000000 to 76.000000.
- * id : factor; set to the value(s): 3. (Might be canceled as random effect, check below.)
- * NOTE : The following random effects columns are canceled: s(id)



Effect of age on arm circumference We can also plot a few of the curves+random effects.

```
mvvlim=c(9.18)
plot_smooth(fit.gamm.reml,view='age',cond=list(id=10),col='orange',ylim=myylim)
plot_smooth(fit.gamm.reml,view='age',cond=list(id=40),col='red',add=TRUE,ylim=myylim)
plot_smooth(fit.gamm.reml,view='age',cond=list(id=120),col='purple',add=TRUE,ylim=myylim)
plot_smooth(fit.gamm.reml,view='age',cond=list(id=50),col='turquoise',add=TRUE,vlim=myylim
```



200