

# 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.

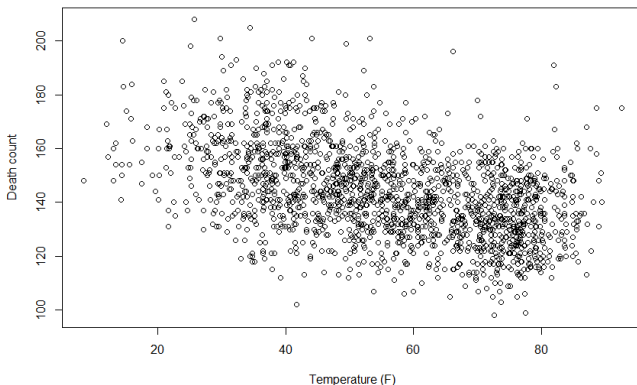
## Concepts

- 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:

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

We can approximate  $g(x_i)$  using

$$g(x_i) = \beta_0 + \beta_1 x_i + \sum_{m=1}^M \beta_{m+1} b_m(x_i)$$

Specify  $b_m(x_i)$ . E.g., linear spline with 9 equidistant interior knots  $\kappa_1, \kappa_2, \dots, \kappa_9$  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:

$$g(x_i) = \beta_0 + \beta_1 x_i + \sum_{m=1}^M \beta_{1+m} b_m(x_i) . \quad (1)$$

Constrain the magnitude of the coefficients  $\beta_j$ .

Consider the **ridge-regression** penalty:

$$\beta_2^2 + \beta_3^2 + \dots + \beta_{M+1}^2 \leq C, \quad (2)$$

equivalently,

$$\|\beta^*\|_2^2 \leq C,$$

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

# Penalties

- Ridge regression = l2-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: convert the two problems of **how many** knots and **where** to put them into a **single parameter** that we can choose.

## Matrix of $g()$

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

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

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

$$\mathbf{G} = \mathbf{X}\beta$$

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



## Constrained formulation

We define the objective function:

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

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

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & \mathbf{0}_{1 \times 40} \\ 0 & 0 & \mathbf{0}_{1 \times 40} \\ \mathbf{0}_{40 \times 1} & \mathbf{0}_{40 \times 1} & \mathbf{I}_{40 \times 40} \end{bmatrix}$$

# Penalized formulation

This problem can be equivalently formulated as

$$\operatorname{argmin}_{\boldsymbol{\beta}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}'\mathbf{B}\boldsymbol{\beta} \quad (3)$$

There is a one-to-one mapping between  $\lambda$  and the constraint  $C$ .  $\lambda$  is often called the **smoothing parameter**.

## Closed-form solution

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

Differentiate wrt  $\boldsymbol{\beta}$  and set to zero:

$$-2\mathbf{X}'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + 2\lambda \mathbf{B}\boldsymbol{\beta} = 0$$

$$-\mathbf{X}'\mathbf{Y} + \mathbf{X}'\mathbf{X}\boldsymbol{\beta} + \lambda \mathbf{B}\boldsymbol{\beta} = 0$$

$$(\mathbf{X}'\mathbf{X} + \lambda \mathbf{B}) \boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{B})^{-1} \mathbf{X}'\mathbf{Y}.$$

## Closed-form solution

The least squares solution is

$$\hat{\beta} = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\mathbf{X}'\mathbf{Y} \quad (4)$$

for some positive number  $\lambda$ . Note:

- When  $\lambda = 0$ ,  $\hat{\beta}$  becomes the ordinary least squares estimate. So no penalization is present ( $C = \infty$ ).
- When  $\lambda \rightarrow \infty$ ,  $(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}$  becomes small, so  $\hat{\beta}_j \rightarrow 0$  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  $\beta_{1+m}, \dots, \beta_{M+1}$  using the **B** matrix:

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & \mathbf{0}_{1 \times 40} \\ 0 & 0 & \mathbf{0}_{1 \times 40} \\ \mathbf{0}_{40 \times 1} & \mathbf{0}_{40 \times 1} & \mathbf{I}_{40 \times 40} \end{bmatrix}$$

# Creating piecewise linear spline

We can create a design matrix with piecewise linear splines.

```
> knots = seq(range(health$Temp)[1], range(health$Temp)[2], length.out = 40+2)
> # place knots evenly on interior of the range of x
> knots = knots[c(2:(length(knots)-1)))]
> X = cbind(rep(1,length(health$Temp)),health$Temp)
> for (i in 1:length(knots)) {
+   X = cbind(X,(health$Temp-knots[i])*(health$Temp>knots[i]))
+ }
> B = diag(42)
> B[1,1]=0
> B[2,2]=0
> dim (X); dim (B)
[1] 1826    42
[1] 42 42
```

# Mortality and Temperature Example

We now search through different values of  $\lambda$ . For each  $\lambda$ , we will

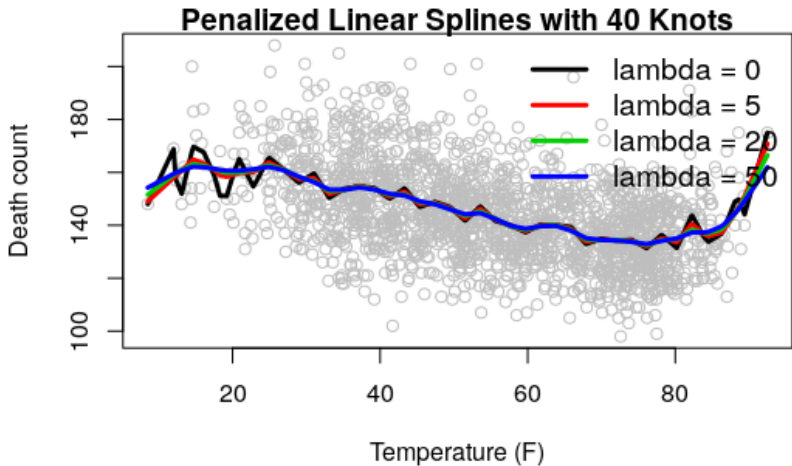
- Calculate the penalized  $\hat{\beta}$ .
- Calculate  $\hat{\beta}' \mathbf{B} \hat{\beta}$ .
- Calculate the fitted value  $\hat{\mathbf{Y}} = \mathbf{X} \hat{\beta}$ .
- Calculate the GCV using the matrix:  $\mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\mathbf{X}'$ .

We will select the  $\lambda$  with the smallest GCV.

```
> Y = health$alldeaths

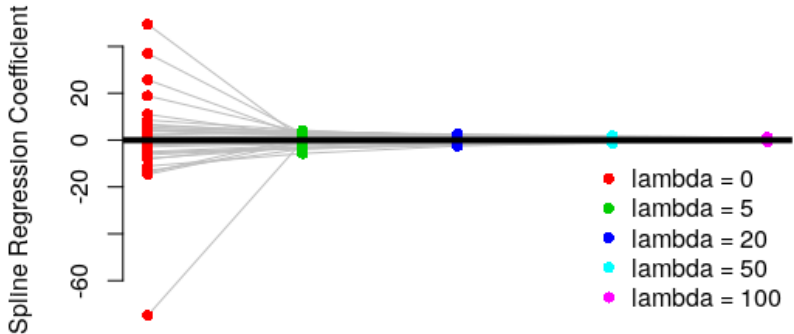
> lambda = 0
> beta = solve (t(X)%*%X + lambda*B) %*% t(X) %*% Y
> H = X %*% solve (t(X)%*%X + lambda*B) %*% t(X)      ##Hat matrix
> Yhat = X%*%beta                                       ##Fitted values
> GCV = mean ( (Y-Yhat)^2 ) / (1- mean (diag(H)))^2
> C = t(beta)%*%B%*%beta
```

## Effects of Penalization





## Effects of Penalization: Shrinkage



# Shrinkage

General principle:

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

How do we determine the tuning parameter  $\lambda$ ?

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  $\hat{\mathbf{Y}} = \mathbf{S}\mathbf{Y}$  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

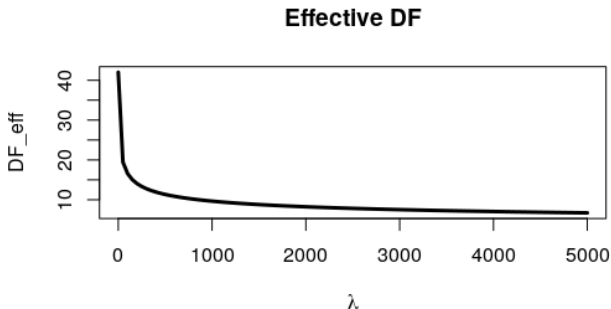
$$\boxed{df_{eff} = tr(\mathbf{S})} . \quad (5)$$

Note: For  $\lambda > 0$ ,  $tr(\mathbf{S}) \neq \text{rank } \mathbf{S}$  because  $\mathbf{S}\mathbf{S} \neq \mathbf{S}$ .  
Hence, “effective” df.

## Effective Degrees of Freedom, cont.

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

As  $\lambda \uparrow$ ,  $df_\lambda \rightarrow 2$  (since  $\beta_0$  and  $\beta_1$  not penalized).



# Generalized Cross-validation Error, revisited

We previously defined GCV:

$$\text{GCV} = \frac{1}{n} \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{[1 - n^{-1} \text{tr}(\mathbf{H})]^2}$$

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

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

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

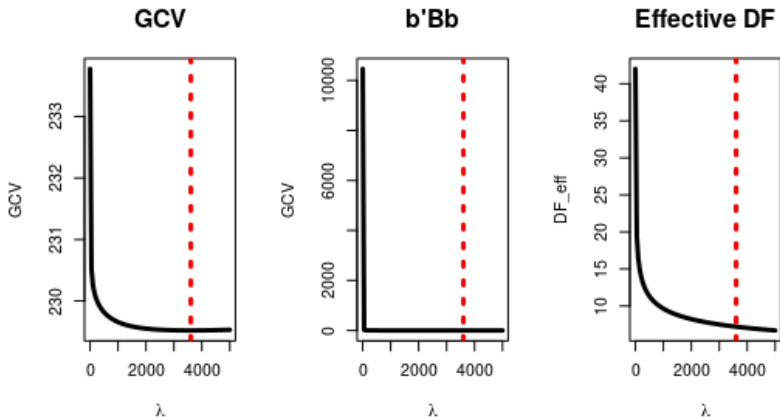
Then GCV is defined:

$$\text{GCV} = \frac{1}{n} \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{[1 - n^{-1} \text{tr}(\mathbf{S})]^2}$$

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

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

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

We have two options:

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

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

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

## 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  $\mathbf{x}'_i$  be the row vector of basis function values for  $x_i$ .

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

$$\begin{aligned} \text{Var}[\hat{g}(x_i)] &= \text{Var}[\mathbf{x}'_i \hat{\boldsymbol{\beta}}] = \mathbf{x}'_i \text{Var}[\hat{\boldsymbol{\beta}}] \mathbf{x}_i \\ &= \mathbf{x}'_i \text{Var}\{(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1} \mathbf{X}'\mathbf{Y}\} \mathbf{x}_i \\ &= \sigma^2 \mathbf{x}'_i (\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1} (\mathbf{X}'\mathbf{X}) (\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1} \mathbf{x}_i . \end{aligned}$$

Note: you should decide whether or not to include the variance due to the intercept. If  $\mathbf{x}_i[1] = 1$ , 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  $\sigma^2$ .

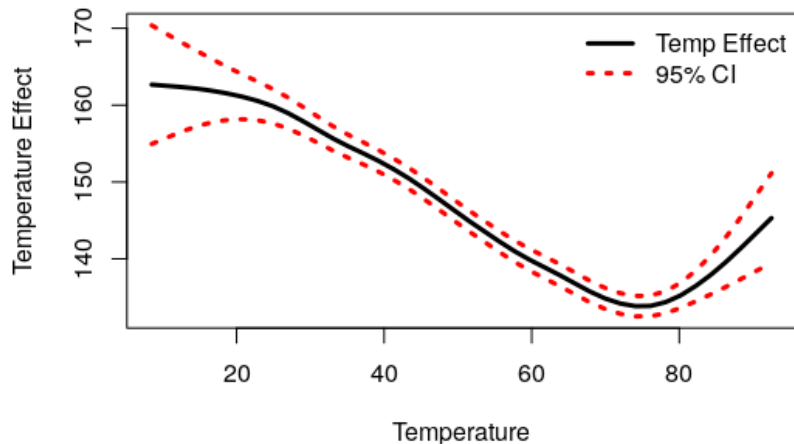
If  $\lambda = 0$ : the previous equation reduces to the OLS variance.

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

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

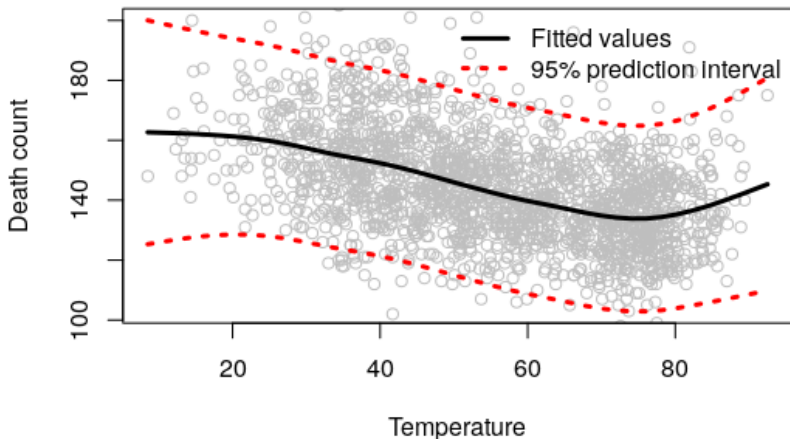
# Temperature Effect on Mortality: pointwise CI

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



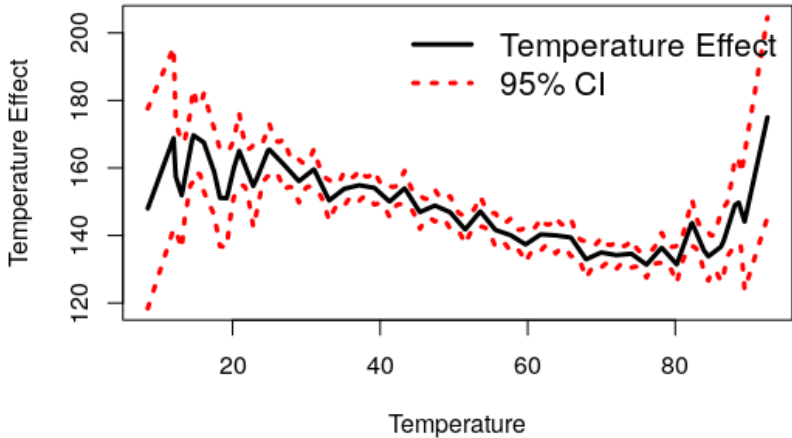
# Daily Mortality Prediction

```
> 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:

$$\hat{g}(x) = \arg \min_{g \in \mathcal{G}} \{\mathbf{Y} - g(\mathbf{x})\}'\{\mathbf{Y} - g(\mathbf{x})\} + \lambda \int_a^b \{g''(x; \boldsymbol{\beta})\}^2 dx. \quad (8)$$

where  $\mathcal{G}$  are twice-differentiable functions,  $\mathbf{x} \in \mathbb{R}^n$  is the vector of  $x_i$ ,  $i = 1, \dots, n$ , and  $a$  and  $b$  is the range of  $x$ .

## Smoothing spline, cont.

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

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

- 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.
- $\lambda$  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

$$(\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta) + \lambda\beta'\mathbf{B}\beta \quad (9)$$

for a certain  $\mathbf{B}$  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  $\mathbf{B}$ .

As before,

- for a given  $\lambda$ , we can estimate  $g(x)$  using penalized least squares;
- search through  $\lambda$  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)
> summary(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 ***

---

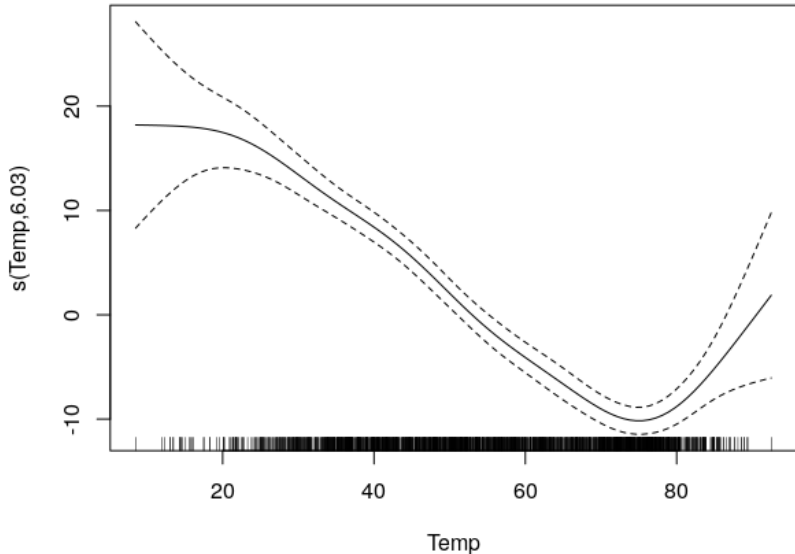
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

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  $2tr(\mathbf{S}) - tr(\mathbf{S}'\mathbf{S})$ .
- Scale est. = estimated residual error  $\sigma^2$  (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 .
```

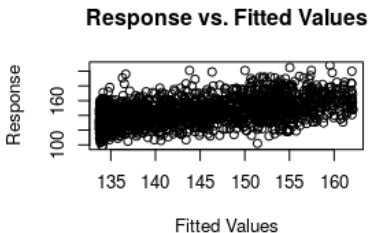
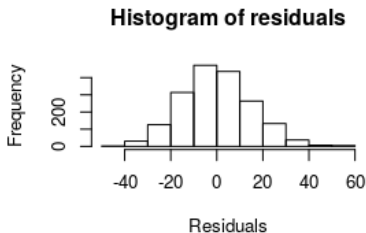
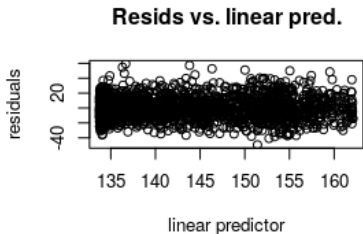
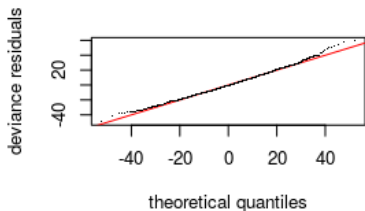
```
The Hessian was positive definite.
```

```
Model rank = 10 / 10
```

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

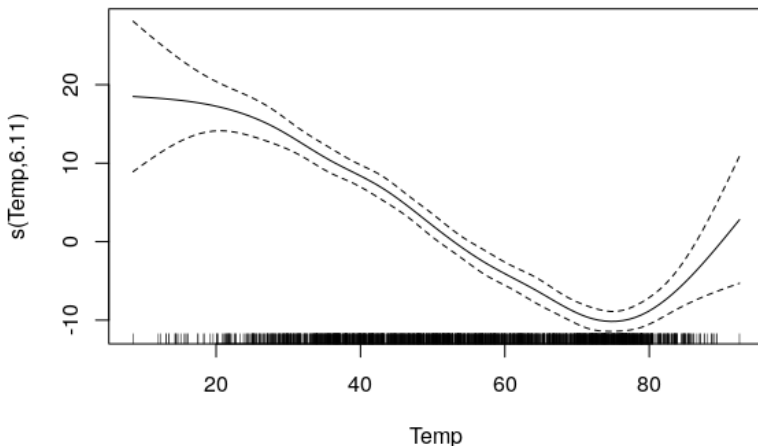
	$k'$	edf	$k\text{-index}$	p-value
s(Temp)	9.00	6.03	1.02	0.88

## gam.check plots



## 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 ~ 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:

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

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

# Mixed model for estimating a penalized spline

Given  $\tau^2$  and  $\sigma^2$ , 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  $\lambda$ .

## 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 )
(Intercept)	143.9168	0.3539	406.7	<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)	5.499	6.665	86.66	<2e-16 ***

---  
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

```
R-sq.(adj) = 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  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ .

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
```

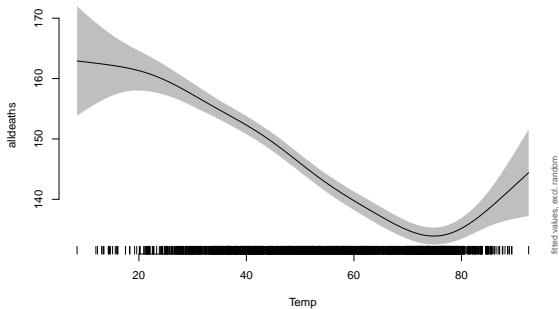
# Interpretation

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:

$$arm_{ij} = \beta_0 + g(age_{ij}) + \theta_i + \epsilon_{ij}$$

$$\theta_i \stackrel{iid}{\sim} N(0, \tau^2)$$

$$\epsilon_{ij} \stackrel{iid}{\sim} N(0, \sigma^2)$$

# 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 894.1436 & scale 0.2364939).
Hessian positive definite, eigenvalue range [1.077516,461.7172].
Model rank = 207 / 207
```

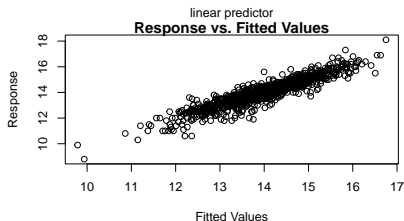
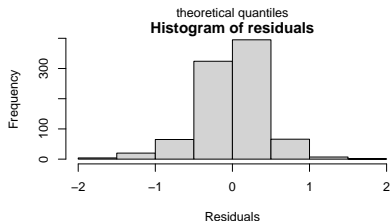
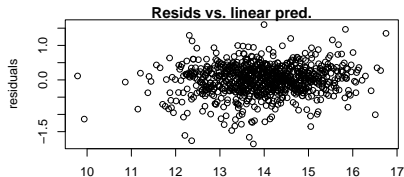
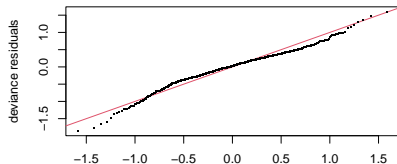
Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

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

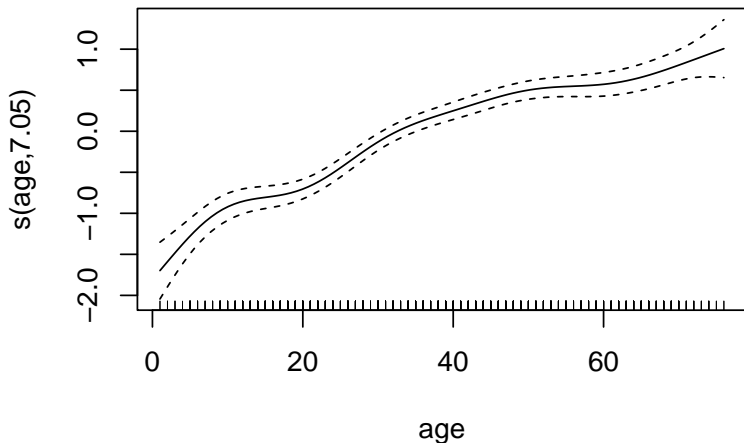
- I tend to prefer REML
- EDF somewhat close to  $k'$ . Other diagnostics okay.
- R code looks at  $k = 20$  and results are similar (edf=8.5), so either this model or the one with  $k = 20$  is fine.
- For random effect,  $k'$  equals number of subjects. Good to check this because will try to fit a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



# Additive mixed model with random intercept



## Effect of age on arm circumference



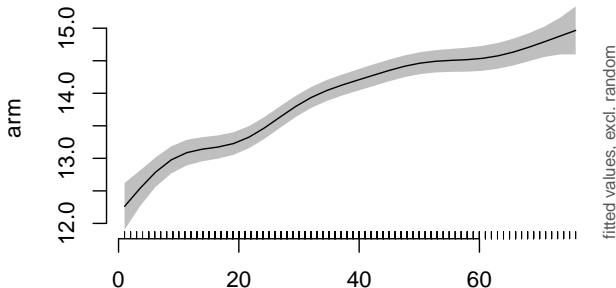
## Effect of age on arm circumference

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.

```
myylim=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,ylim=myylim)
```

