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.

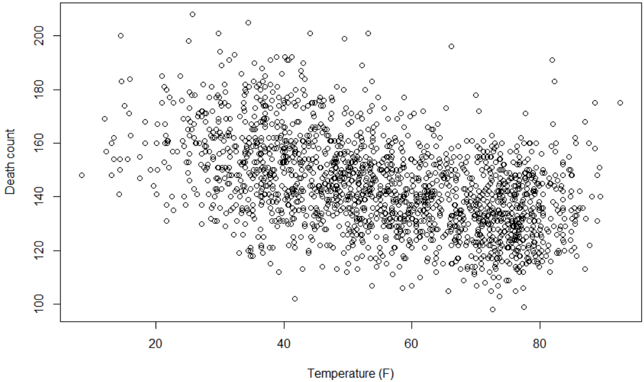
Concepts

- 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:

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

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 $\kappa_1, \kappa_2, \ldots, \kappa_9$ within the observed range of daily temperature, a piecewise linear spline model is

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

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:

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

Constrain the magnitude of the coefficients β_j.

Consider the ridge-regression penalty:

$$\beta_2^2 + \beta_3^2 + \ldots + \beta_{M+1}^2 \leq C, \tag{2}$$

equivalently,

$$||\boldsymbol{\beta}^*||_2^2 \leq C,$$

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

Penalties

- Ridge regression = l2-penalty = $||\boldsymbol{\beta}^*||_2^2$.
- Other penalties: lasso = absolute value = l1-penalty = $||\boldsymbol{\beta}^*||_1 = \sum_{j=2}^{M+1} |\beta_j|$.
- 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, $i = 1, \ldots, n$:

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

Then write $g(x_i)$, $i = 1, \ldots, n$ 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:

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

Here, $\mathbf{B}$ 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

$$\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \; (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}'\mathbf{B}\boldsymbol{\beta} \tag{3}$$

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

Closed-form solution

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

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

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

Closed-form solution

The least squares solution is

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

for some positive number λ. Note:

- When $\lambda = 0$, $\hat{\boldsymbol{\beta}}$ 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:

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

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

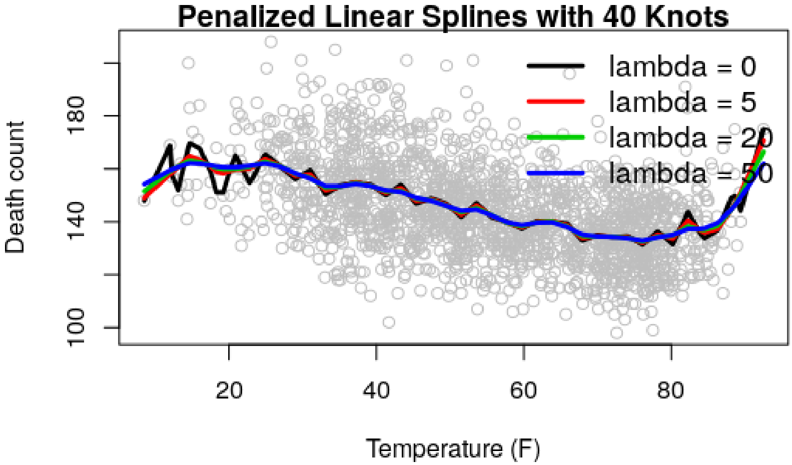
We now search through different values of λ. For each λ, we will

- Calculate the penalized $\hat{\boldsymbol{\beta}}$.
- 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: $\mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\mathbf{X}'$.

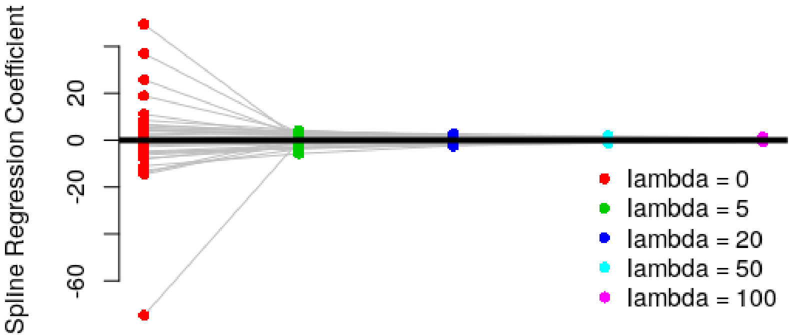
We will select the λ with the smallest GCV.

```
> 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 $\rightarrow$ $\downarrow$ variance.
- $\uparrow$ shrinkage $\rightarrow$ $\uparrow$ 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 $\hat{\mathbf{Y}} = \mathbf{S}\mathbf{Y}$ 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

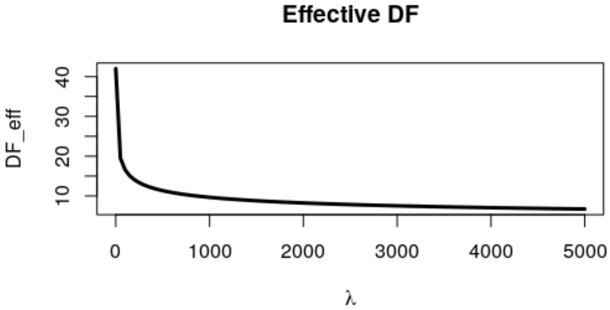
$$\boxed{df_{eff} = tr(\mathbf{S})}\,. \tag{5}$$

Note: For $\lambda > 0$, $tr(\mathbf{S}) \neq \mathrm{rank}\,\mathbf{S}$ because $\mathbf{SS} \neq \mathbf{S}$.
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 $\lambda \uparrow$, $df_\lambda \to 2$ (since β_0 and β_1 not penalized).



Generalized Cross-validation Error, revisited

We previously defined GCV:

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

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 $\mathbf{Y}$ that can be written in the form:

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

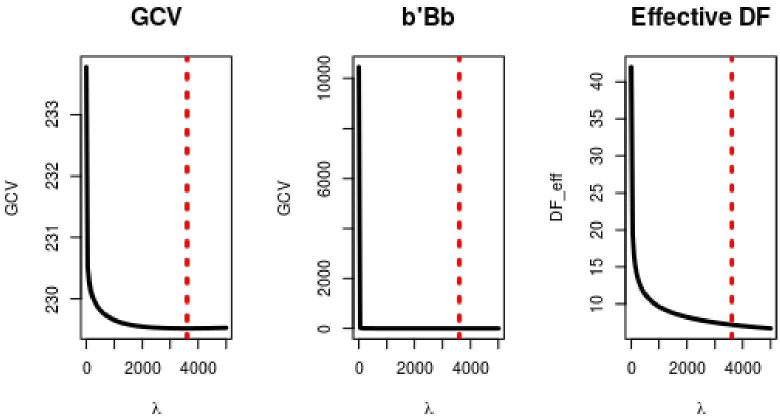
Then GCV is defined:

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

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

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

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

We have two options:

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

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

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

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

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

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

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

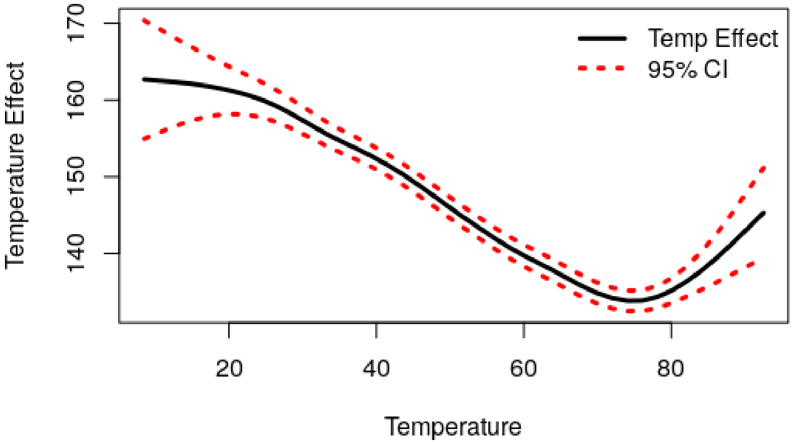
If $\lambda = 0$: the previous equation reduces to the OLS variance.

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

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

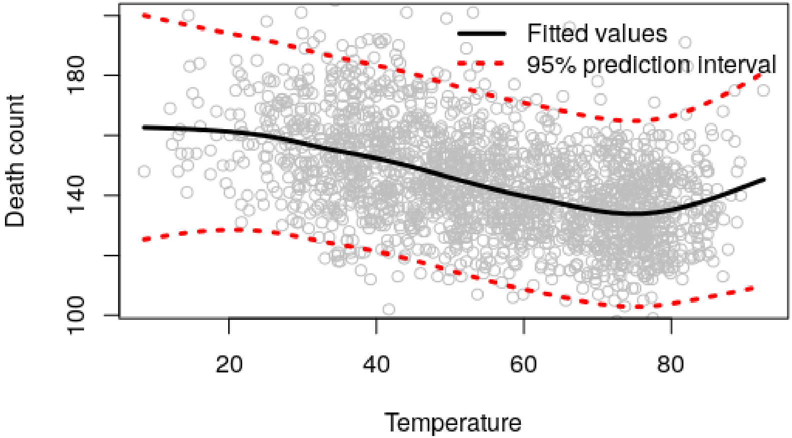
Temperature Effect on Mortality: pointwise CI

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



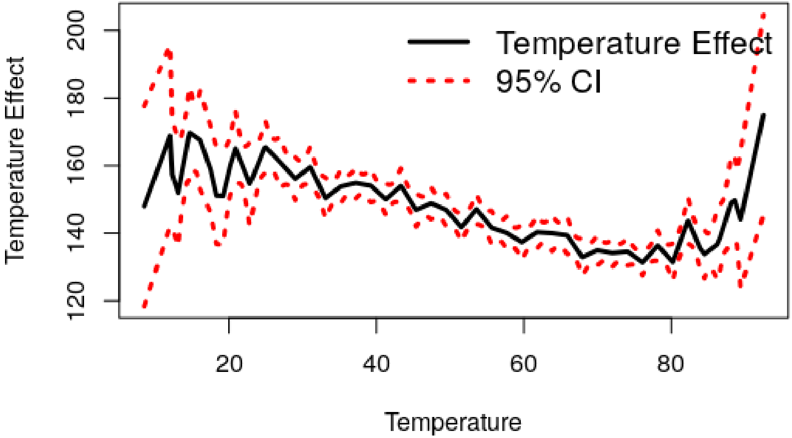
Daily Mortality Prediction

```
> 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:

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

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

Smoothing spline, cont.

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

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

- 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

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

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. min edf=1 (unpenalized linear term, if edf=1, results nearly equivalent to lm()).
- Selection methods (default: GCV).
- Family (default: Gaussian).
- Standard error computation (default: Bayesian).

Temperature Effect on Mortality

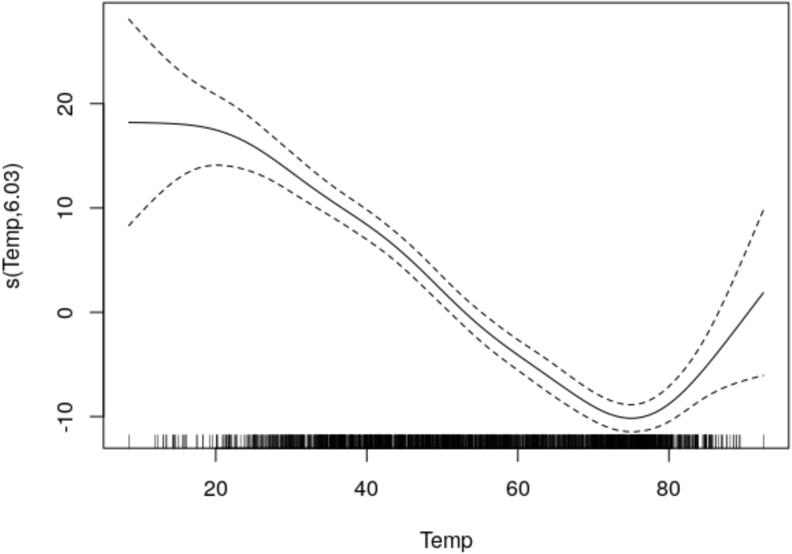
```
> library (mgcv)
> fit1 = gam(alldeaths~s(Temp), data= health)
> summary(fit1)

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 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



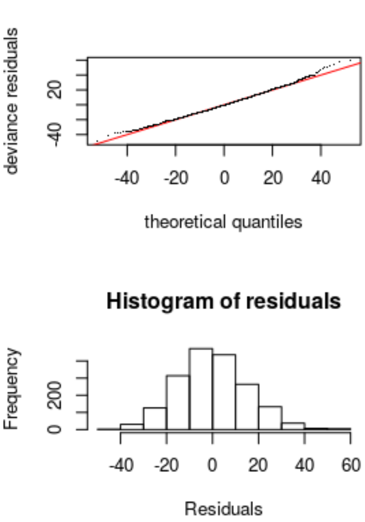
Checking gam

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

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

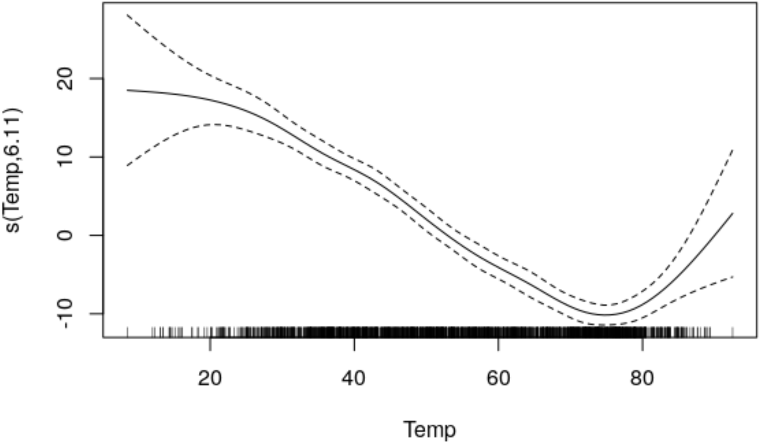
```
Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 5 iterations.
The RMS GCV score gradient at convergence was 7.242e-05 .
The Hessian was positive definite.
Model rank =  10 / 10

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



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:

$$y_i = \beta_0 + \beta_1 x_i + \sum_{m=1}^{M} \theta_m (x_i - \kappa_m)_+ + \epsilon_i,$$

$$\theta_m \overset{iid}{\sim} N(0, \tau^2), \quad \epsilon_i \overset{iid}{\sim} N(0, \sigma^2)$$

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

Mixed model for estimating a penalized spline

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

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

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|)
(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
```

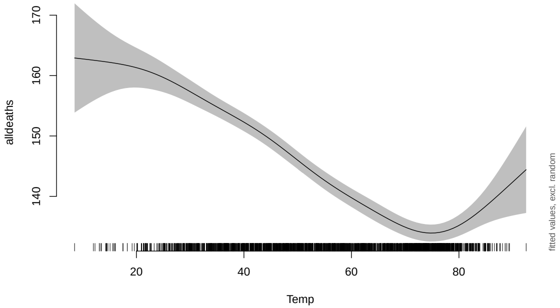
Interpretation

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:

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

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

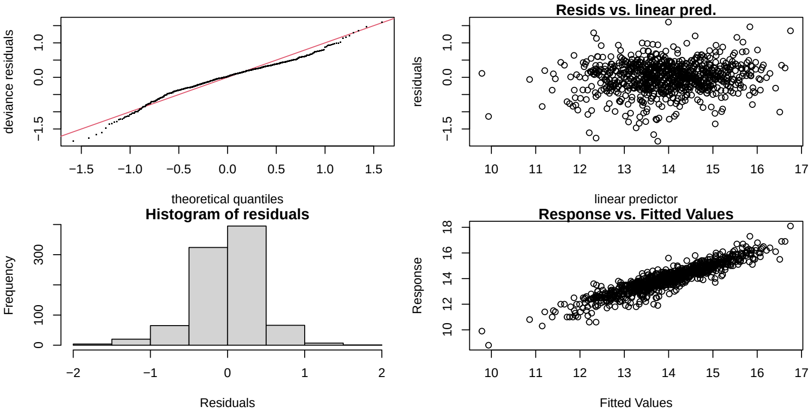
$$\epsilon_{ij} \overset{iid}{\sim} N(0, \sigma^2)$$

Additive model with random intercept

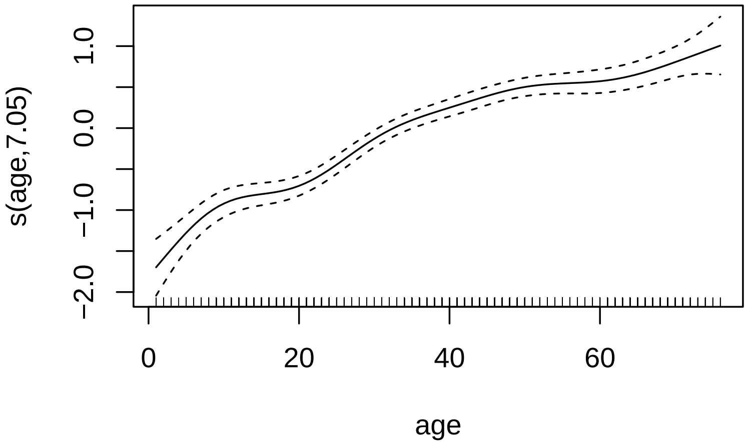
```
 fit.gamm = gam(arm~s(age)+s(id,bs = 're'),method='REML',data=nepal)
> gam.check(fit.gamm)

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



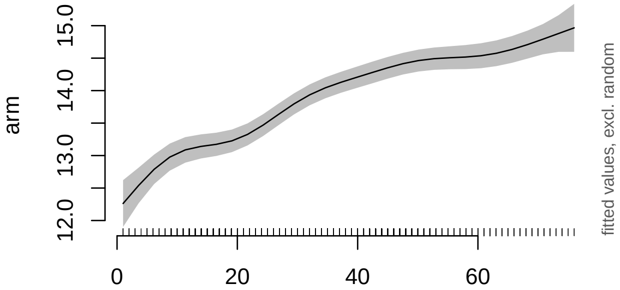
Effect of age on arm circumference



Effect of age on arm 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.

```
 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)
```