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.

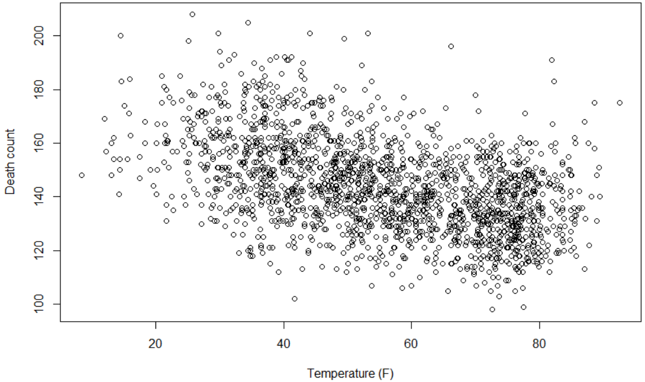
Concepts

- 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 $g(\cdot)$ using

E.g., 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:

Constrain the magnitude of the coefficients β_j.

Consider the ridge-regression penalty:

equivalently,

where C is an unknown positive constant.

Penalties

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

Penalized Spline

Equations (1) and (2) can be written in matrix form:

Here, **B** is a diagonal matrix with 0 and 1 entries selecting which coefficients are penalized, defined below.

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

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

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

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 $\hat{\boldsymbol{\beta}} \to \mathbf{0}$.

Mortality and Temperature Example

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

$$y_i = \beta_0 + \beta_1 x_i + \sum_{m=1}^{40} \beta_{2+m} \left(x_i - \kappa_m\right)_+$$

The constraint implies a **B** matrix:

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

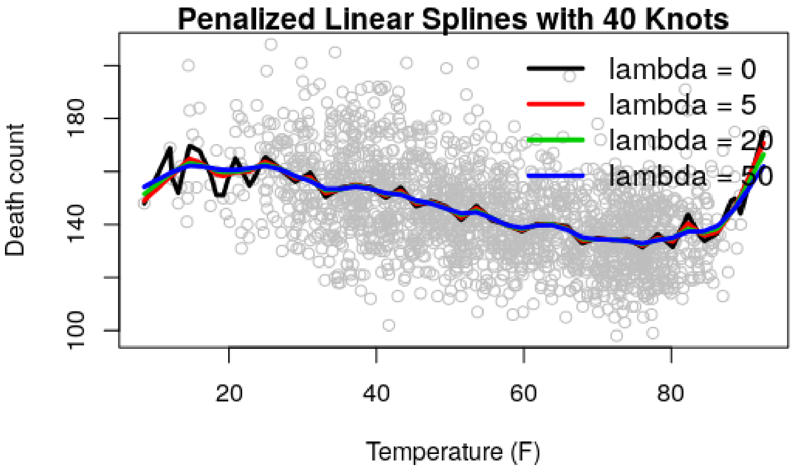
We now search through different values of λ. For each λ, we will

- 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: $\mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\mathbf{X}'$.

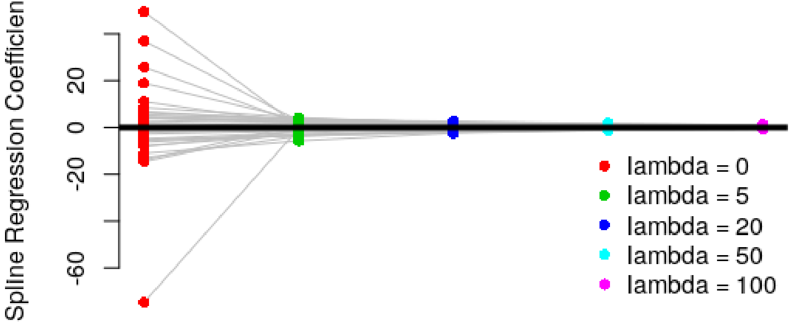
We will select the λ with the smallest GCV.

```
> 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 $\rightarrow$ 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 $\hat{\mathbf{Y}} = \mathbf{S}\mathbf{Y}$ 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

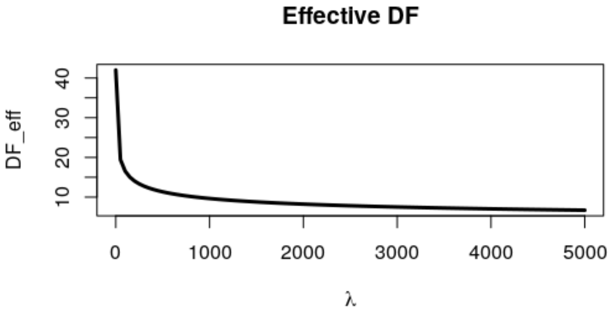
$$\boxed{\qquad\qquad\qquad} \,. \tag{6}$$

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 $\lambda \uparrow$,



Generalized Cross-validation Error, revisited

We previously defined GCV:

$$\boxed{\text{GCV} = \qquad\qquad\qquad\qquad}$$

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:

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

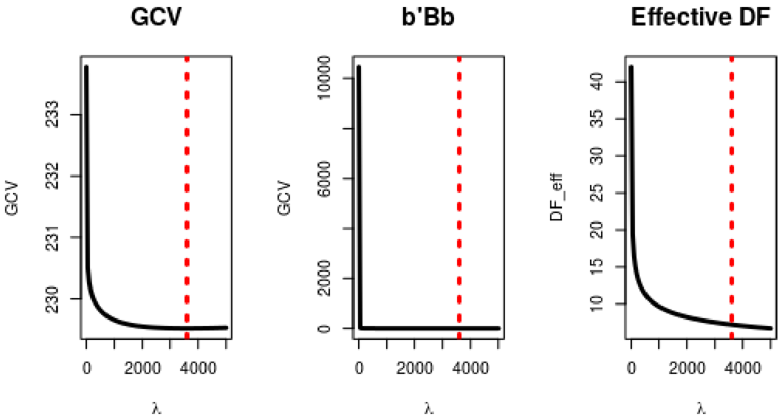
Then GCV is defined:

$$\boxed{\text{GCV} = \qquad\qquad\qquad\qquad}$$

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:

$$\boxed{\hat{\sigma}^2 = \frac{\displaystyle\sum_{i=1}^{n} [y_i - \hat{g}(x_i)]^2}{n - df_{\text{eff}}}}. \tag{7}$$

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

$$\boxed{\hat{\sigma}^2_{\text{unbiased}} = \frac{\displaystyle\sum_{i=1}^{n} [y_i - \hat{g}(x_i)]^2}{n - 2\text{tr}\{\mathbf{S}\} + \text{tr}\{\mathbf{S}\mathbf{S}'\}}}. \tag{8}$$

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

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.

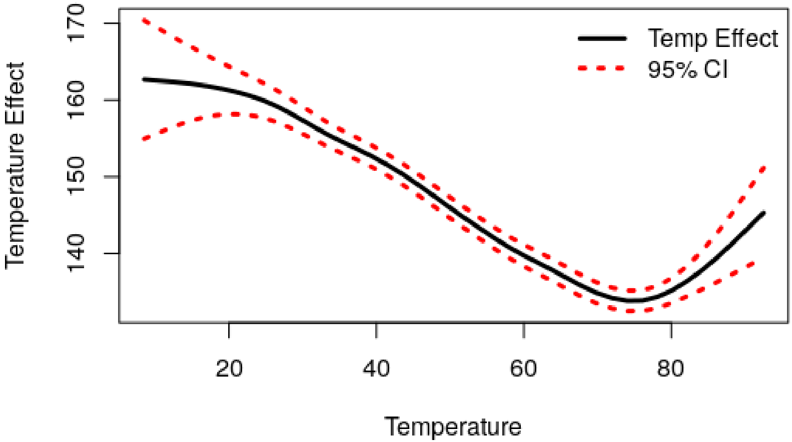
If $\lambda = 0$:

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

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

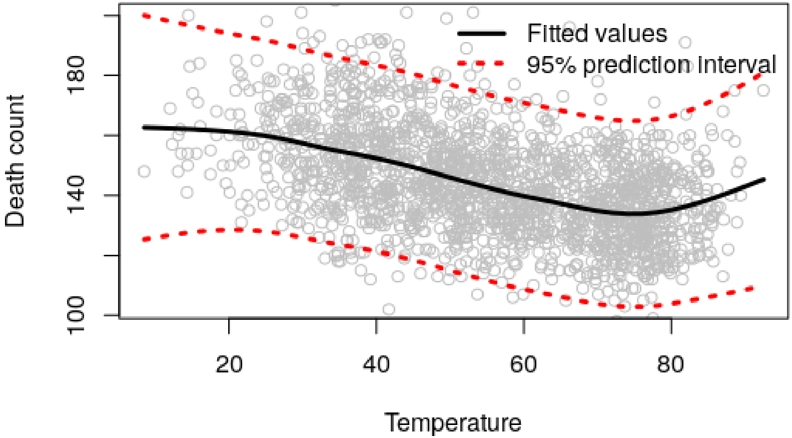
Temperature Effect on Mortality: pointwise CI

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



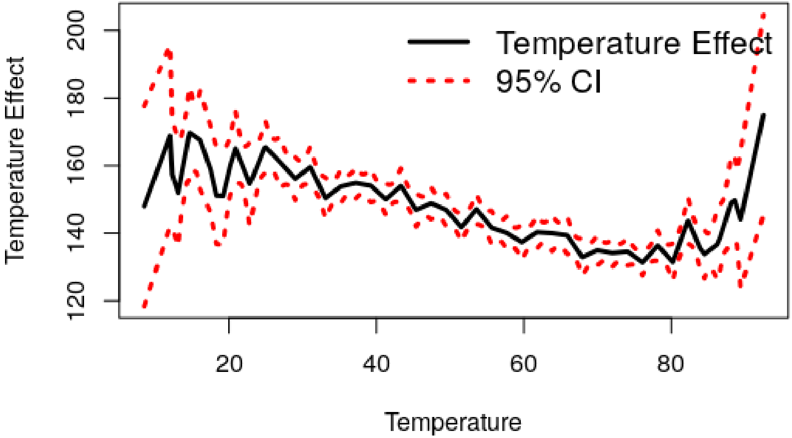
Daily Mortality Prediction

```
> 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.

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

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 (9) 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 (10) 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

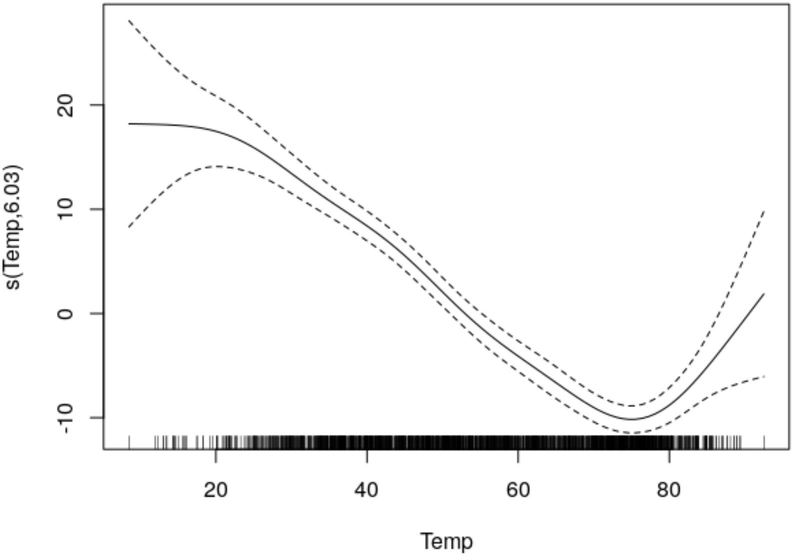
```
> library (mgcv)
> fit1 = gam(alldeaths~s(Temp), data= health)
> summary(fit1)

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



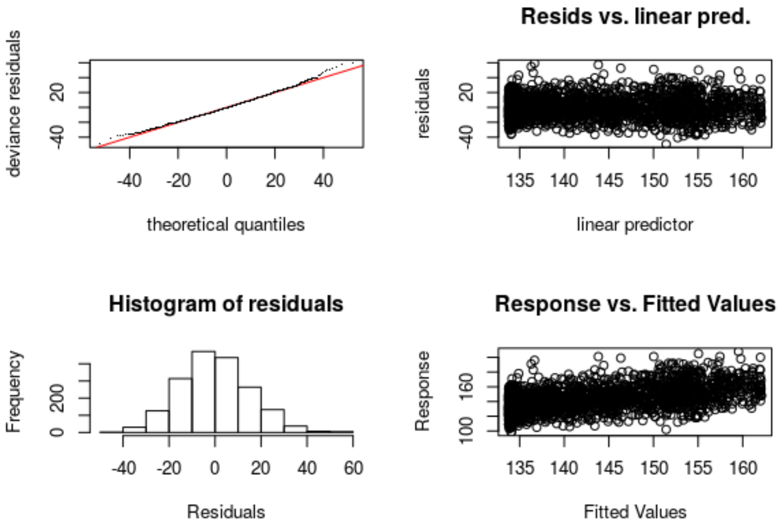
Checking gam

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

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

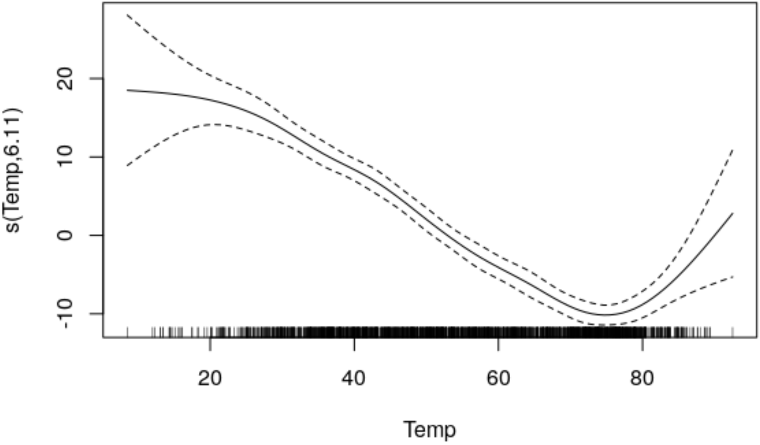
```
Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 5 iterations.
The RMS GCV score gradient at convergence was 7.242e-05 .
The Hessian was positive definite.
Model rank =  10 / 10

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:

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

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

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

Mixed model for estimating a penalized spline

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

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

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) with a slight decrease in the number of deaths until approximately 30 degrees. The deaths decrease at a relatively constant rate from approximately 30 to 75 degrees. For example, 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 95 degrees, the number of deaths increases by approximately 0.8 for every 1 degree increase in temperature.

Additive model with random intercept

Recall the Nepal arm circumference dataset.

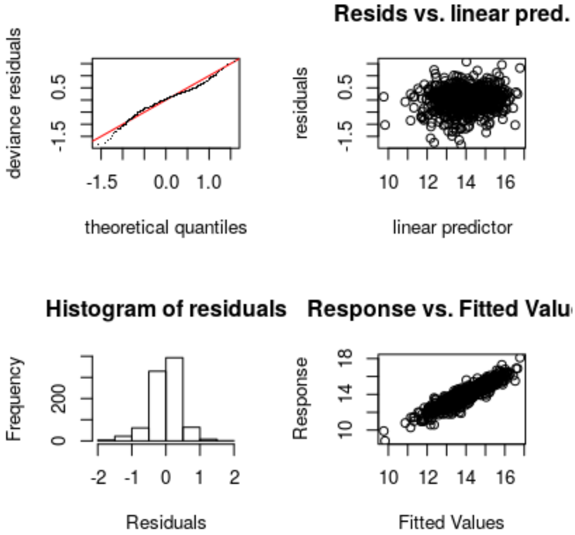
Data on 200 children collected at a maximum of 5 time points about 4 months apart.

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

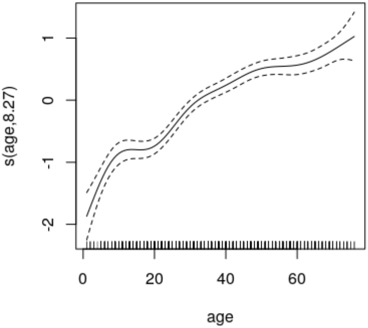
Additive model with random intercept

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

Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 5 iterations.
The RMS GCV score gradient at convergence was 1.71e-06 .
The Hessian was positive definite.
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   8.27    1.03    0.83
s(id)  197.00 183.32      NA      NA
```

Additive mixed model with random intercept



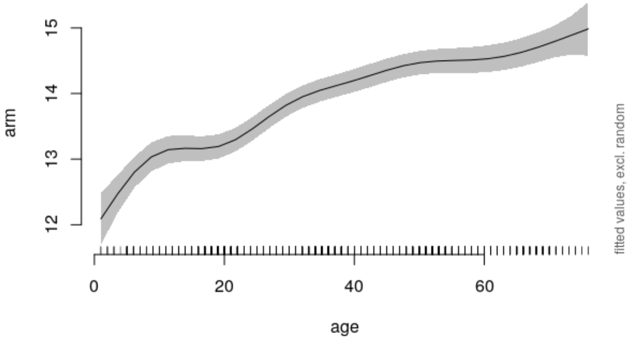
Effect of age on arm circumference



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)
```