Module 5 Part 2: Penalized Splines

Wednesday, November 1, 2023 14:21

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5_PartII_...

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.

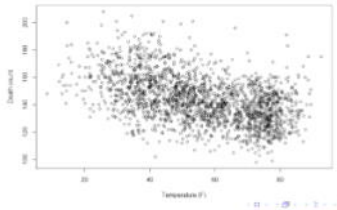
Concepts

- 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 a generalized additive model

$$y_i = g(x_i) = \beta_0 + \beta_1 x_i + \sum_{m=1}^{M} \beta_{m+1} b_m(x_i) \qquad \epsilon_i \overset{iid}{\sim} (0, \sigma^2)$$

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: (too many)

- 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.

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will limit β's so not too big → prevent overfitting & collinearity

Penalized Spline

Consider the basis expansion: β_{1+m} = β_{m+1}

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

Constrain the magnitude of the coefficients β_j.

Consider the ridge-regression penalty:

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

equivalently, (all the betas excluding β_0 and β_1)

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

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

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Penalties

Lasso & Ridge

"L"

- 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. W/ GCV

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Ridge regression: introduce bias to decrease variance

↓

minimizes residuals AND λ * slope^2 ?

(As opposed to OLS which just minimizes residuals)

It's better to standardize variables before applying ridge bc it's squared so scale matters

Lasso regression: minimizes residuals AND λ * |slope|

→ ↑ λ, β goes all the way to 0, unlike ridge regression, where they will approach 0

∴ lasso can get rid of useless variables like histological sign

Matrix of g()

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

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

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

$$\mathbf{G} = \mathbf{X}\boldsymbol{\beta}, \quad g(x_i) = \beta_0 + \beta_1 x_i + \sum_{m=1}^{M} \beta_{m+1} (x_i - \kappa_i)_+$$

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

aka $b_i(x_i)$

8/32 Module 5, part II: Penalized and Smoothing Splines

Constrained formulation

↳ if you don't want to penalize all the β's

We define the objective function:

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

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

not penalize intercept
not penalize global term

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

aka

0 0 0
0 0 0
0 0 1
1 1 ...

then $\beta'\mathbf{B}\beta = \sum_{m=2}^{M+1} \beta_M^2$

Penalized formulation

This problem can be equivalently formulated as

$$\underset{\beta}{\text{argmin}} \ (\mathbf{Y}-\mathbf{X}\beta)'(\mathbf{Y}-\mathbf{X}\beta) + \lambda\beta'\mathbf{B}\beta \qquad (3)$$

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

→ can be 0 to ∞

when estimating a spline

↓

tuning parameter
hyperparameter

Closed-form solution

noted:

$\frac{d}{d\beta}(y-X\beta)^2$

$\sim 2X(y-X\beta)$

won't need to derive on exam

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

Differentiate wrt β and set to zero:

$$-2\mathbf{X}'(\mathbf{Y}-\mathbf{X}\beta) + 2\lambda\mathbf{B}\beta = 0$$
$$-\mathbf{X}'\mathbf{Y} + \mathbf{X}'\mathbf{X}\beta + \lambda\mathbf{B}\beta = 0$$
$$(\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})\beta = \mathbf{X}'\mathbf{Y}$$
$$\hat{\beta} = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{B})^{-1}\mathbf{X}'\mathbf{Y}.$$

$(X'X+\lambda\beta)^{-1}X'Y$

Closed-form solution

penalized least squares, not ordinary least squares

The least squares solution is

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

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 $B_{jj} = 1$. → so slope gets smaller

aka

↑ λ, ↓ slope

here, $\hat{\beta}_0$ and $\hat{\beta}_1$ are not penalized

but the non-linear parts of the spines (coefs corresponding to knots)

go to 0 as $\lambda \to \infty$

How do we pick λ?
Use cross-validation,
typically 10-fold cross validation
look at the one with least
residual variance aka MSE

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 $\mathbf{B}$ matrix:

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

so $\beta'\mathbf{B}\beta = \sum_{m=1}^{40} \beta_{1+m}^2$

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:

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

so $\beta' \mathbf{B} \beta = \sum_{m=1}^{40} \beta_{1+m}^2$

13/32

Use cross-validation, typically 10-fold cross validation. Look at the one with least residual variance aka MSE

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
```

14/32

Mortality and Temperature Example

We now search through different values of λ. For each λ, 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 λ with the smallest GCV.

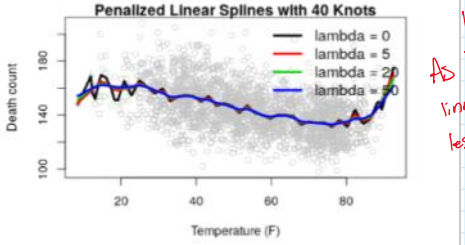
Use GCV

```
> 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
```

loop over all values of λ in the code, you can plot what things look like

15/32

Effects of Penalization

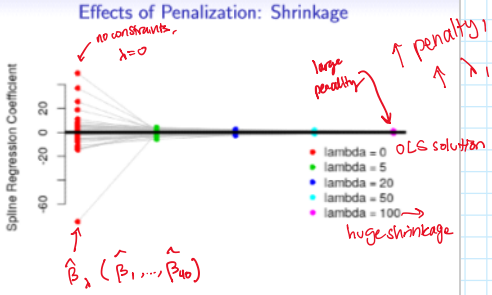


16/32

Heavier penalty

As $\lambda \uparrow$, line becomes less wiggly, betas go towards 0?

Effects of Penalization: Shrinkage



no constraints, $\lambda = 0$

large penalty

OLS solution

huge shrinkage

$\hat{\beta}_\lambda \; (\hat{\beta}_1, \ldots, \hat{\beta}_{40})$

↑ penalty, ↑ λ, coefficients → 0

Shrinkage

less wiggly

$\hat{g}$ are based on data Y

General principle:

- ↑ shrinkage → ↓ variance.
- ↑ shrinkage → ↑ bias.

$E\left[\hat{g}(x_i) - \epsilon(\hat{g}(x_i))\right]^2$

$\left[g(x_i) - E(\hat{g}(x_i))\right]^2$

How do we determine the tuning parameter λ?

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

GCV

at some point you're oversmoothing ↓ just fitting mean

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

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

$\sum_{i=j} S_{ij}$ aka the diagonals

Note: For $\lambda > 0$, $tr(\mathbf{S}) \neq \text{rank } \mathbf{S}$ because $\mathbf{SS} \neq \mathbf{S}$.
Hence, "effective" df: effective # of parameters

OLS: $S = X(X'X)^{-1}X'$ $SS = S$ i.e. idempotent

therefore $tr(S) = \text{rank}(S) = df = n - p$

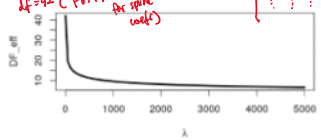
Ridge: $SS \neq S$, replace df with EFFECTIVE DF $= tr(S)$

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).

huge λ=0 has df = 42 ($\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_{42}$ for spline coefs)



$= B$

Generalized Cross-validation Error, revisited

We previously defined GCV:

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

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:

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

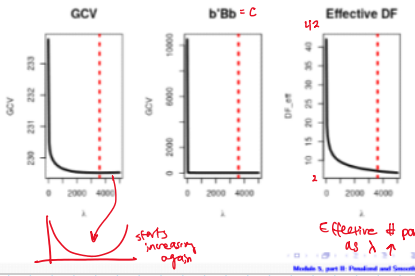
Then GCV is defined:

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

This is the definition we will use hereafter.

Smoothing Parameter Selection

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



starts increasing again

Effective # parameters ↓ as λ ↑

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:

mgcv:: gam

e.df

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

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

Ref. df

Will see this later in mgcv package in R

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

↳ in OLS, $n - 2p + p = n - p$ ✓

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

$\tilde{x}_i = (1, x_i, x_i - k_1)_+, \ldots, (x_i - k_{40})_+)$

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

$= \tilde{x}_i' [X'X + \lambda B]^{-1} X' \, Var(Y) \, [X(X'X + \lambda B)^{-1}] \tilde{x}_i$

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.

confusing whether $\hat{g}(x_i)$ includes β_0. MGCV:: gam does not include $\hat{\beta}_0$

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.

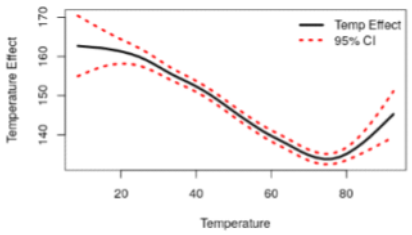
Similarly the variance for an unobserved point y_i^* with covariate x_i^* has variance new value of $(y_i^*, \hat{x}_i^*)$

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

↳ same as previous slide, just add additional σ^2

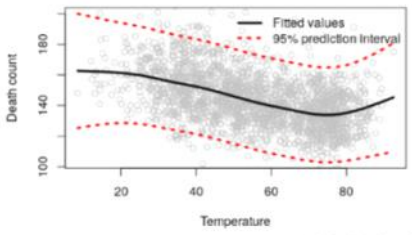
Temperature Effect on Mortality: pointwise CI

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



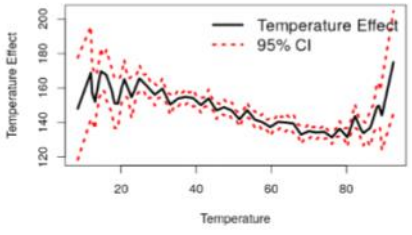
Daily Mortality Prediction

```
> 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

NOT PART OF EXAM

Smoothing splines: specify df rather than λ?

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:

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

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.

29/52 Module 5, part B: Penalized and Smoothing Splines

Smoothing spline, cont.

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

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.

30/52 Module 5, part B: Penalized and Smoothing Splines

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

basis expansion of x

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

for a certain $\mathbf{B}$ matrix based on second moments of the basis functions, no longer diagonal; see Ruppert et al p. 75. → semiparametric regression

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

31/52 Module 5, part B: Penalized and Smoothing Splines

Note: another package called GAM but not as good

Package mgcv in R → WILL BE ON EXAM

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()). 10 parameters - 1 constraint = 9 free parameters
- Selection methods (default: GCV).
- Family (default: Gaussian).
- Standard error computation (default: Bayesian).

32/52 Module 5, part B: Penalized and Smoothing Splines

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
```

approximate F statistic if edf=1, simplifies to usual t-statistic

33/52

mgcv::gam output

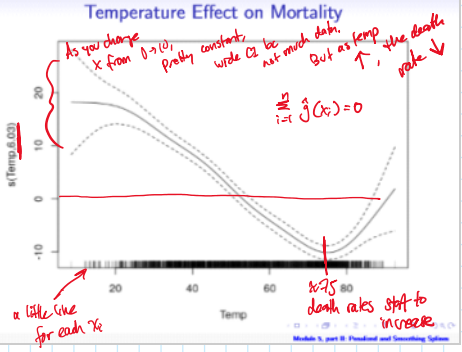
```
Approximate significance of smooth terms:
          edf Ref.df    F p-value
s(Temp) 6.03    7.2 80.6  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.241   Deviance explained = 24.3%
GCV = 229.47  Scale est. = 228.58    n = 1826
```

$\hat{\sigma}^2$

- 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 $\hat{g}(x_i)$.

34/52

Temperature Effect on Mortality



As you change X from 1 → 10, pretty constant, wide CI bc not much data. But as temp ↑, the death rate ↓

$\sum_{i=1}^{n} \hat{g}(x_i) = 0$

a little like for each x_i

death rates start to increase

35/52

Checking gam

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

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

function we use to get diagnostics plots

```
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
```

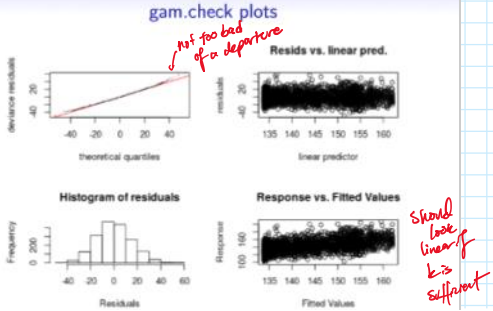
H_0: Basis dimension is adequate – This test not very useful

In general, "k" should be "notably" larger than edf e.g. edf ≤ 5, here we will check fitting model w/ a higher basis dimension

36/52

gam.check plots

not too bad of a departure



should look linear if k is sufficient

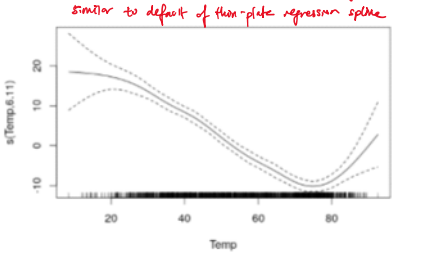
shows look linear if k is sufficient

37/52

Temperature Effect on Mortality using cubic

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

Checks to see if a diff spline impacts things here, similar to default of thin-plate regression spline



38/52

(informal sensitivity analysis to basis dimension)

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
```

edf only increased a little
k=10 is sufficient

39/52

Extract Useful Model Statistics

Full list see ?gamObject.

- AIC (with edf at penalized estimates)

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

- Variance-covariance matrix of the coefficients of your spline basis

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

(not really; they have frequentist coverage probabilities, so we default to using these)

- Fitted value

```
> fit$fitted
```

40/52

A different approach to smoothing rather than GCV

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:

(or whatever basis you are using)

- Applies to non-clustered data (though you could use clustered?)
- smoothing title

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

random slope

Data is not longitudinal here so this is a little fishy

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

↑ wiggly ↑ τ^2
↑ noisy ↑ σ^2

↳ becomes larger with more wiggly data

↳ becomes larger with more noisy data → if $\sigma^2 >> \tau^2$ then we will get ...?

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

41/52

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.

$$\|Y - X\beta - Z\theta\|^2 + \frac{\sigma^2}{\tau^2}\|\theta\|_2^2$$

if τ^2 is very large → large penalty → shrink coefs towards 0

Selecting penalty using mixed models

- In mgcv::gam, we can use the option `method='REML'`
- Often results in greater smoothing (smaller effective degrees of freedom)

```
> 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?

$\hat{g}'(40)$

```
> # 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.

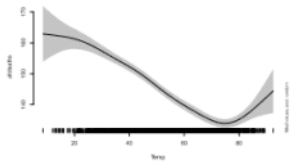
Deaths are highest at cold temperatures (< 10 degrees F) and slightly decreasing until approximately 20 degrees. Then deaths decrease at a similar rate from approximately 25 to 75 degrees. The number of deaths decreases by approximately 0.5 people / degree in a neighborhood of 40 degrees. Then the number 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.

$\hat{g}'(40)$

$\hat{g}'(85)$

g(x) Interpretation

from 'mgcv' package



Additive model with random intercept

GAMM: generalized additive mixed model

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:

$$arm_{ij} = \beta_0 + g(age_{ij}) + \theta_i + \epsilon_{ij}$$
$$\theta_i \overset{iid}{\sim} N(0, \tau^2)$$
$$\epsilon_{ij} \overset{iid}{\sim} N(0, \sigma^2)$$

$\theta_i \perp \epsilon_{ij}$

Additive model with random intercept

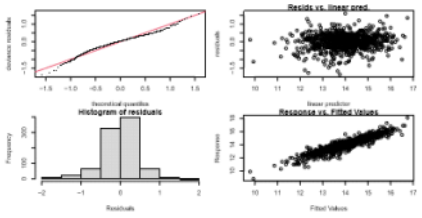
```
fit_gamm = gam(arm~s(age)+s(id,bs = 're'),method="REML",data=nepal)
> gam.check(fit_gamm)

Method: REML   Optimizer: outer newton
full convergence after 6 iterations.
Gradient range [ -4.190347e-07, -5.779523e-08]
(score 994.1836 & scale 0.2368893).
Hessian positive definite, eigenvalue range [1.077516,461.71772].
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    1.01    0.79
s(id) 199.00 81.63      NA      NA
```

s(id) ↔ # participants (-1?)

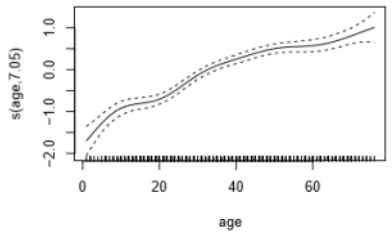
→ MGCV tests random effects in an annoying way but these actually $\hat{\theta}_i$ from random intercept

- 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

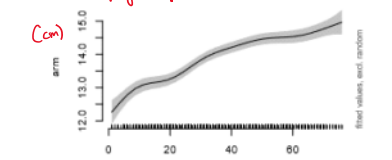
This plot includes the intercept:

```
> 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)
```

Estimate of population trajectory

no random effects?

(cm)



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
```

$\hat{\beta}_0 + \hat{g}(age_i) + \hat{\theta}_i$