Functional Response Models

Response is a set of curves $y_i(t)$ $i = 1, \ldots, n$.

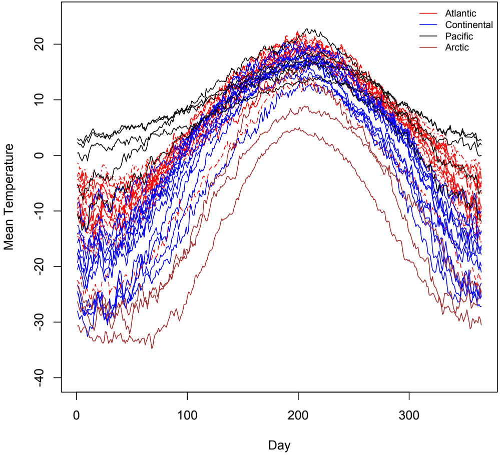
Covariates may be

- group labels
- scalar values
- functions

Today we will focus on the first two.

Functional ANOVA

Is there a difference between regions?



Regional Effects

Just as in the standard ANOVA, let

$$x_{ij}(t) = i\text{th curve in } j\text{th group}$$

with n_j curves in group j.

- An over-all mean

$$\bar{x}(t) = \frac{1}{\sum n_j} \sum_{j=1}^{K} \sum_{i=1}^{n_j} x_{ij}$$

- effects for each group

$$\alpha_j(t) = \frac{1}{n_j} \sum_{i=1}^{n_j} \left(x_{ij}(t) - \bar{x}(t) \right)$$

- an error process

$$\epsilon_{ij}(t) = x_{ij}(t) - \alpha_j(t) - \bar{x}(t)$$

General Scalar Covariates

ANOVA Model

$$x_{ij}(t) = \mu(t) + \alpha_j(t) + \epsilon_{ij}(t)$$

Suppose we observe scalar covariates $z_{i1}, \ldots, z_{ip}$, $i = 1, \ldots, n$

The functional model is

$$y_i(t) = \beta_0(t) + \sum_{j=1}^{p} \beta_j(t) z_{ij} + \epsilon_i(t)$$

and we assume that the $\epsilon_i(t)$ are random error processes with at least

$$E\epsilon_i(t) = 0$$

That is, we now have coefficient *functions*.

Fitting a Model by Least Squares

At each time t we have

$$y_i(t) = \mathbf{z}_i \beta(t) + \epsilon_i(t)$$

so we can solve the least-squares equations to get

$$\beta(t) = (Z^T Z)^{-1} Z^T \mathbf{y}(t)$$

But we would like to represent $\beta(t)$ as a functional data object.

Basis Expansions

More generally, we want to represent

$$\beta_j(t) = \Phi_j(t)\mathbf{c}_j$$

then we need a new least-squares criterion:

$$\text{SSE}(\beta) = \sum_{i=1}^{n} \int (y_i(t) - \mathbf{z}_i\beta(t))^2 \, dt$$

if the $y_i(t)$ and the $\beta(t)$ share the same basis, this is exactly the same as the point-wise solution.

However, sometimes we may want to make the $\beta(t)$ smoother.

Some Mechanics

$$\text{SSE}(\beta) = \sum_{i=1}^{n} \int (y_i(t) - \mathbf{z}_i \beta(t))^2 \, dt$$

write

$$\mathbf{b} = [\mathbf{c}_1^T \ \cdots \ \mathbf{c}_p^T]^T$$

and

$$\Psi_i(t) = [z_{i1}\Phi_1(t) \ \cdots \ z_{ip}\Phi_p(t)]$$

then

$$\hat{\mathbf{b}} = \left[\sum \int \Psi_i(t)\Psi_i(t)^T dt\right]^{-1} \left[\sum \int \Psi_i(t)^T y_i(t) dt\right]$$

Mechanics for the Functional ANOVA

$$x_{ij}(t) = \mu(t) + \alpha_j(t) + \epsilon_{ij}(t)$$

Requires a constraint:

$$\sum_{j=1}^{k} \alpha_j(t) = 0, \ \forall t$$

Incorporated automatically in most software.

`fda` library requires manual support

Mechanics for the Functional ANOVA

To make this work for us:

$$Z = \text{indicator matrix}, \mathbf{z}_i^* = [1 \ Z_i]$$

Define a new observation

$$\mathbf{z}_{n+1} = [0 \ 1 \ \cdots 1], \ y_{n+1}(t) = 0$$

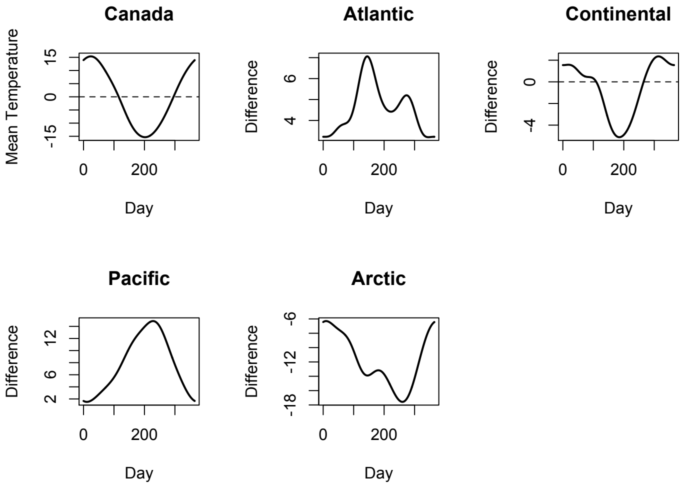
then fit

$$y_i(t) = \mathbf{z}_i \beta(t) + \epsilon_i(t)$$

Results in

$$\mu(t) = \beta_1(t), \ \alpha_j(t) = \beta_{j+1}(t)$$

Temperature Data



Significance

To test significance, we can define a pointwise F-statistic

$$F(t) = \frac{\text{Var}(\hat{\mathbf{y}}(t))}{\sum (y_i - \hat{y}_i)^2}$$

indicates where there is a large amount of signal relative to noise.

Test over-all regression significance based on

$$F^* = \max F(t)$$

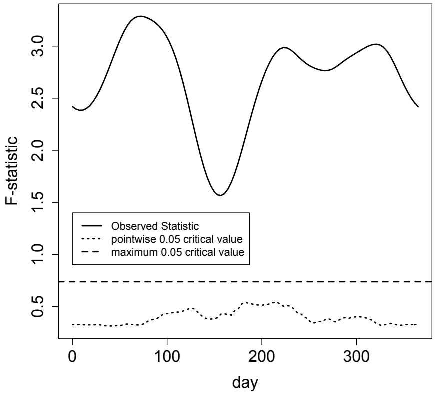
Permutation Test: $H_0 : \beta_j(t) = 0$ for all $j = 1, \ldots, p$, $\forall$ t.

Do B times

1. Permute the indeces $1, \ldots, n$ to get $i_1, \ldots, i_n$
2. Define $y_j^b(t) = y_{i_j}(t)$
3. Estimate the model using $\mathbf{y}^b(t)$ as the response.
4. Measure F_b^*.

If $\frac{1}{B} \sum_{b=1}^{B} I(F^* - F_b^*) > \alpha$ reject $H_0 : \forall t : Ey(t) = 0$

Test for Regional Effects



Smoothing and Functional Response Models

In addition to estimating the model, we may also want to smooth.

Usual smoothing method:

$$\mathrm{PENSSE}_\lambda(\beta) = \sum \int (y_i(t) - \mathbf{z}_i \beta(t))^2 \, dt + \sum_j \lambda_j \int [L_j \beta_j(t)]^2 \, dt$$

But, $\beta_j(t)$ is defined without smoothing. Why would we want to?

Reduction in variance due to

1. high-frequency noise-process in the $\epsilon_i(t)$.
2. correlation across the $\epsilon_i(t)$.

Basically: if we think the $\beta(t)$ are smooth, we should use that information!

Mechanics

Recall from regression with scalar responses that

$$\sum_j \lambda_j \int [L_j \beta_j(t)]^2 \, dt = \mathbf{b}^T \begin{bmatrix} \lambda_1 R_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_p R_p \end{bmatrix} \mathbf{b} = \mathbf{b}^T R \mathbf{b}$$

with

$$R_j = \int L\Phi_j(t) L\Phi_j(t)^T dt$$

then

$$\hat{\mathbf{b}} = \left[\sum \int \Psi_i(t)\Psi_i(t)^T dt + R \right]^{-1} \left[\sum \int \Psi_i(t)^T y_i(t) dt \right]$$

Cross Validation

We can select the amount of smoothing by leave-one-curve out cross validation.

$\hat{\beta}_\lambda^{-i}(t)$ is the model estimated without $y_i(t)$.

Then we choose λ to minimize

$$\text{CV}(\lambda) = \sum \int \left(y_i(t) - \mathbf{z}_i \hat{\beta}_\lambda^{-i}(t) \right)^2 dt$$

This can be written down in terms of matrices like usual OCV, but it is not implemented in the `R` library.

There is no equivalent definition of GCV.

Summary

- Functional responses regressed on scalar covariates $\Rightarrow$ just linear regression at each time t.
- Basis expansions make things more interesting
- Permutation F tests for over-all significance.