## P-spline mixed models for spatio-temporal data

María Durbán joint work with Dae-Jin Lee

DEPARTMENT OF STATISTICS UNIVERSIDAD CARLOS III DE MADRID

June 2009

## **Outline**

1 P-splines

Mixed models approach Multidimensional *P*-splines

2 P-splines for spatial count data

Spatial smoothing
Smooth-CAR model
Application: Scottish Lin Cance

Application: Scottish Lip Cancer data

Spatio-temporal data Smoothing with P-splines ANOVA-Type Interaction Models Application Environmental spatio-temporal data

**4** Spatio-temporal Disease Mapping

## **Outline**

## 1 P-splines

Mixed models approach Multidimensional *P*-splines

P-splines for spatial count data

Spatial smoothing
Smooth-CAR model
Application: Scottish Lip Cancer data

3 Spatio-temporal data Smoothing with P-splines ANOVA-Type Interaction Models Application Environmental spatio-temporal data

Spatio-temporal Disease Mapping

### ▶ Penalized Likelihood splines (Eilers & Marx, 1996):

- Given the data  $(x_i, y_i)$ , i = 1, ..., n
- Fit a sum of local basis functions:

$$\mathbf{y}_i = f(\mathbf{x}_i) + \boldsymbol{\epsilon}_i, \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{\sigma}^2)$$

where 
$$f(x_i) = B\theta$$
 and

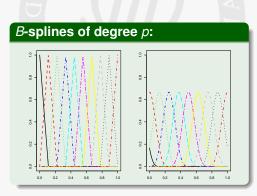
- ▶ B = B(x) is a **Regression Basis**, and
- $\triangleright$   $\theta$  is a vector of **coefficients**.
- Control the fit through a smoothing parameter (λ).

<sup>»</sup> Regression Basis

"The Flexible Smoother"

### ▶ B-splines Basis:

- p + 1 Piece-wise polynomials of degree p.
- Connected by knots.
- In general the choice is p=3, cubic spline.



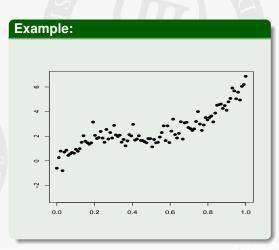
## ▶ B-splines Basis:

• 
$$\widehat{y} = f(x_i) = B\widehat{\theta}$$

• B-splines Regression

Optimal selection of knots (Complet).

 P-Spines: add a penalty to control smoothness.



» Methodolo

## ▶ B-splines Basis:

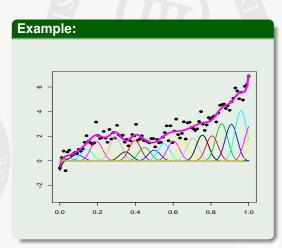
• 
$$\widehat{y} = f(x_i) = B\widehat{\theta}$$

**B**-splines Regression:

$$\min S(\theta; y) = \|y - B\theta\|^2$$

$$\widehat{\theta} = (B'B)^{-1}B'y$$

- Optimal selection of knots (Complex).



## ▶ B-splines Basis:

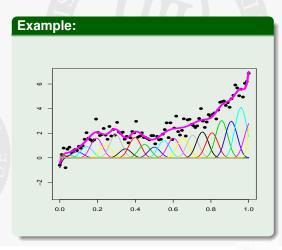
• 
$$\widehat{y} = f(x_i) = B\widehat{\theta}$$

**B**-splines Regression:

$$\min S(\theta; y) = \|y - B\theta\|^2$$

$$\widehat{\theta} = (B'B)^{-1}B'y$$

- Optimal selection of knots (Complex).
- P-Splines: add a penalty to control smoothness.



#### Methodology:

Minimize the penalized sum of squares (PSS):

$$S(\theta; y, \lambda)_p = \|y - B\theta\|^2 + \mathsf{PENALTY}$$

- The **PENALTY** term, controls the smoothness of the fit by  $\lambda$ 
  - ► Eilers & Marx (1996):
    - $\Rightarrow$  (discrete) **Penalty** over adjacent coefficients  $\theta$ .
  - ► Lang & Brezger (2004):
    - $\Rightarrow$  "Bayesian *P*-splines": random walk priors for  $\theta$ , e.g.:

$$m{ heta} |m{ heta}_{m-1} \sim \mathcal{N}(m{ heta}_{m-1}, au^2), ext{ or } \ m{ heta} |m{ heta}_{m-1}, m{ heta}_{m-2} \sim \mathcal{N}(2m{ heta}_{m-1} - m{ heta}_{m-2}, au^2)$$

María Durhán

#### Methodology:

Minimize the penalized sum of squares (PSS):

$$S(\theta; y, \lambda)_p = \|y - B\theta\|^2 + \mathsf{PENALTY}$$

- The PENALTY term, controls the smoothness of the fit by λ.
  - ► Eilers & Marx (1996):
    - $\Rightarrow$  (discrete) **Penalty** over adjacent coefficients  $\theta$ .
  - ► Lang & Brezger (2004):
    - $\Rightarrow$  "Bayesian *P*-splines": random walk priors for  $\theta$ , e.g.:

$$m{ heta} | m{ heta}_{m-1} \sim \mathcal{N}(m{ heta}_{m-1}, au^2), ext{ or } \ m{ heta} | m{ heta}_{m-1}, m{ heta}_{m-2} \sim \mathcal{N}(2m{ heta}_{m-1} - m{ heta}_{m-2}, au^2)$$

#### Methodology:

Minimize the penalized sum of squares (PSS):

$$S(\theta; y, \lambda)_p = \|y - B\theta\|^2 + PENALTY$$

- The PENALTY term, controls the smoothness of the fit by λ.
  - ► Eilers & Marx (1996):
    - $\Rightarrow$  (discrete) **Penalty** over adjacent coefficients  $\theta$ .
  - ▶ Lang & Brezger (2004):
    - $\Rightarrow$  "Bayesian *P*-splines": random walk priors for  $\theta$ , e.g.:

$$\boldsymbol{\theta} | \boldsymbol{\theta}_{m-1} \sim \mathcal{N}(\boldsymbol{\theta}_{m-1}, \tau^2), \text{ or }$$

$$\boldsymbol{\theta}|\boldsymbol{\theta}_{m-1},\boldsymbol{\theta}_{m-2} \sim \mathcal{N}(2\boldsymbol{\theta}_{m-1}-\boldsymbol{\theta}_{m-2},\tau^2)$$

#### PSS becomes:

$$S(\theta; y, \lambda)_p = ||y - B\theta||^2 + \theta' P\theta$$

- $ightharpoonup P = \lambda D'D.$
- $ightharpoonup \lambda$  is the smoothing parameter.
- ▶ D are difference matrices.
- For given  $\lambda$  ,  $\min S(\theta; y, \lambda)_p$

$$\widehat{\boldsymbol{\theta}} = \left( \boldsymbol{B}' \boldsymbol{B} + \lambda \boldsymbol{D}' \boldsymbol{D} \right)^{-1} \boldsymbol{B}' \boldsymbol{y}$$

 $ightharpoonup \lambda$  can be selected by CV, GCV, AIC or BIC.

PSS becomes:

$$S(\theta; y, \lambda)_p = ||y - B\theta||^2 + \theta' P\theta$$

- $ightharpoonup P = \lambda D'D.$
- $ightharpoonup \lambda$  is the smoothing parameter.
- ▶ D are difference matrices.
- For given  $\lambda$ , min  $S(\theta; y, \lambda)_p$

$$\widehat{\boldsymbol{\theta}} = (\boldsymbol{B}'\boldsymbol{B} + \lambda \boldsymbol{D}'\boldsymbol{D})^{-1}\boldsymbol{B}'\boldsymbol{y}$$

 $ightharpoonup \lambda$  can be selected by CV, GCV, AIC or BIC.

PSS becomes:

$$S(\theta; y, \lambda)_p = ||y - B\theta||^2 + \theta' P\theta$$

- $ightharpoonup P = \lambda D'D.$
- λ is the smoothing parameter.
- ▶ D are difference matrices.
- For given  $\lambda$ ,  $\min S(\theta; y, \lambda)_p$

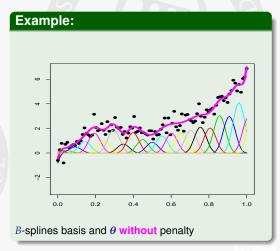
$$\widehat{\boldsymbol{\theta}} = (\boldsymbol{B}'\boldsymbol{B} + \lambda \boldsymbol{D}'\boldsymbol{D})^{-1}\boldsymbol{B}'\boldsymbol{y}$$

 $\blacktriangleright$   $\lambda$  can be selected by CV, GCV, AIC or BIC.

"The Flexible Smoother"

### ▶ 1*d P*-splines:

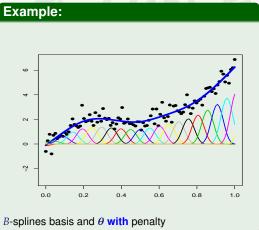
- No penalty over coefficients.
- Penalty over coefficients.



"The Flexible Smoother"

### ▶ 1*d P*-splines:

- Penalty over coefficients.



"The Flexible Smoother"

#### Advantages over other smoothers:

- Low-Rank: "dim(B) < dim(data)".
- Computationally efficient: "# knots ≤ 40".
- Selection of number and Location of knots is NOT and issue.
- Discrete Penalties over the  $\theta$ , not over the fitted curve.
- Easy extension to:
  - ▶ Mixed models.
  - non-gaussian data (GLM's) and
  - Multidimensional smoothing.
  - Spatial and Spatio-temporal smoothing.

Miyed model

A mixed model approach

#### ▶ Reformulate:

• Model  $y = B\theta + \epsilon$ , into

$$y = X\beta + Z\alpha + C\alpha$$

where x and Z are "fixed" and "random" effects matrice

with coefficients G and  $G \sim \mathcal{N}(0, G)$ , and

#### A mixed model approach

#### ► Reformulate:

• Model  $y = B\theta + \epsilon$ , into

$$y = X\beta + Z\alpha + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I)$$

- ▶ where X and Z are "fixed" and "random" effects matrices.
- lacktriangle with coefficients eta and  $m{lpha}\sim\mathcal{N}(0,m{G})$ , and  $m{G}=m{\sigma}_{m{lpha}}^2m{R}$

#### A mixed model approach

Reparameterization:

$$B \equiv [X : Z] \Rightarrow B\theta = X\beta + Z\alpha$$

 $\blacktriangleright$  We use the Singular Value Decomposition (SVD) on D'D

» SVE

#### ► Singular Value Decomposition (SVD)

$$D'D = U\Sigma U'$$

• with  $\boldsymbol{U} = [\boldsymbol{U}_n : \boldsymbol{U}_s]$ 

$$D'D = [U_n : U_s] \left[ \begin{array}{c|c} \mathbf{0}_d & \\ & \widetilde{\Sigma} \end{array} \right] \left[ \begin{array}{c|c} U'_n \\ \hline U'_s \end{array} \right]$$

- $\Sigma \equiv \text{non-null eigenvalues}$ .
- ▶  $U_n$  = eigenvectors corresponding to the null eigenvalues.
- $ightharpoonup U_s \equiv$  eigenvectors corresponding to the non-null eigenvalues.

#### A mixed model approach

- The fix effects (β) are unpenalized and
- The **Penalty**  $\theta'P\theta$  becomes

$$\alpha' F \alpha$$

where  $F = \lambda \widetilde{\Sigma}$  is diagonal.

And the random effects (α) covariance matrix G:

$$G = \sigma^2 F^{-1}$$

Mixed Model Basis:

$$X = [1:x]$$

$$Z = BU_s$$

A mixed model approach

#### Advantages:

- Flexibility:
  - ► Easy incorporation of smoothing in complex models ("spatial" random effects and/or correlated errors).
- Mixed Models Theory:
  - Estimation and Inference.
- Software Implementation.
  - R, Splus, MATLAB or SAS.
- Extension to non-gaussian data:
  - ► Generalized Linear Mixed Models (GLMM)

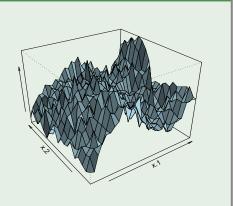
#### Example: 2d-array

- Data  $Y = y_{ij}$ ,  $i = 1, ..., n_1$  and  $j = 1, ..., n_2$
- Array structure:  $n_1$  rows and  $n_2$  columns

$$Y = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n_2} \\ y_{21} & y_{22} & \cdots & y_{2n_2} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n_11} & \cdots & \cdots & y_{n_1n_2} \end{bmatrix}$$

Regressors:

$$x_1 = (x_{11}, \dots, x_{1n_1})'$$
  
 $x_2 = (x_{21}, \dots, x_{2n_2})'$ 

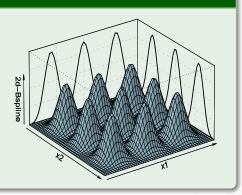


▶ Use of Tensor Products of *B*-splines (Durbán et al, 2002):

#### Example: 2d-array

- Marginal Basis:
  - $B_1 = B_1(x_1)$ , of dim.  $n_1 \times c_1$ .
  - $B_2 = B_2(x_2)$ , of dim.  $n_2 \times c_2$ .
- 2d B-splines Basis:
  - Kronecker Product (⊗) of marginal basis:

$$B = B_2 \otimes B_1$$
, of dim.  $n_1 n_2 \times c_1 c_2$ 

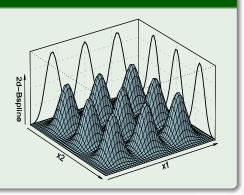


▶ Use of Tensor Products of *B*-splines (Durbán et al, 2002):

#### Example: 2d-array

- Marginal Basis:
  - $B_1 = B_1(x_1)$ , of dim.  $n_1 \times c_1$ .
  - $B_2 = B_2(x_2)$ , of dim.  $n_2 \times c_2$ .
- 2d B-splines Basis:
  - Kronecker Product (⊗) of marginal basis:

$$B = B_2 \otimes B_1$$
, of dim.  $n_1 n_2 \times c_1 c_2$ 



#### Model:

$$y = f(x_1, x_2) + \epsilon,$$

with  $y_{n_1n_2\times 1}$ 

• In matrix form,  $\hat{y} = B\theta$  can be written as:

$$\widehat{\mathbf{Y}} = \mathbf{\textit{B}}_1 \mathbf{\textit{A}} \mathbf{\textit{B}}_2, \text{ of dim } n_1 \times n_2$$

where A is a matrix  $c_1 \times c_2$  of coefficients  $\theta$  of length  $c_1c_2 \times 1$ .

#### IDEA:

- Set penalties over Θ.
  - Row-wise Penalty:

$$oldsymbol{ heta}'\left(oldsymbol{I}_{c_2}\otimes oldsymbol{D}_1'oldsymbol{D}_1
ight)oldsymbol{ heta}$$

• Column-wise Penalty:

$$heta' \left( oldsymbol{D}_2' oldsymbol{D}_2 \otimes oldsymbol{I}_{c_1} 
ight) heta$$

#### Model:

$$y = f(x_1, x_2) + \epsilon,$$

with  $y_{n_1 n_2 \times 1}$ 

• In matrix form,  $\hat{y} = B\theta$  can be written as:

$$\widehat{\mathbf{Y}} = \mathbf{B}_1 \mathbf{A} \mathbf{B}_2$$
, of dim  $n_1 \times n_2$ 

where A is a matrix  $c_1 \times c_2$  of coefficients  $\theta$  of length  $c_1c_2 \times 1$ .

#### **IDEA:**

- Set penalties over Θ.
  - Row-wise Penalty:

$$oldsymbol{ heta}'\left(oldsymbol{I}_{c_2}\otimesoldsymbol{D}_1'oldsymbol{D}_1
ight)oldsymbol{ heta}$$

• Column-wise Penalty:

$$oldsymbol{ heta}' \left( oldsymbol{D}_2' oldsymbol{D}_2 \otimes oldsymbol{I}_{c_1} 
ight) oldsymbol{ heta}$$

► Penalty Matrix in 2d:

$$P = \lambda_1 \underbrace{I_{c_2} \otimes D_1' D_1}_{P_1} + \lambda_2 \underbrace{D_2' D_2 \otimes I_{c_1}}_{P_2}$$

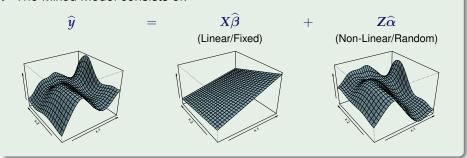
- $\lambda_1$  and  $\lambda_2$  are the smoothing parameters in each dimension.
- Anisotropy:  $(\lambda_1 \neq \lambda_2)$

**Mixed Models Representation** 

► As in 1d Case:

### **Example:**

► The Mixed Model consists of:



#### ► Mixed Models Representation:

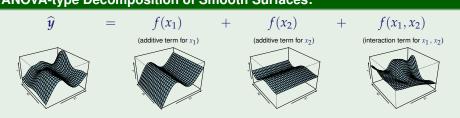
• As in 1d case, the aim is:

$$B \equiv [X : Z] \Longrightarrow B\theta = X\beta + Z\alpha$$

- The SVD over P allows the simultaneous diagonalization of  $D_1'D_1$  and  $D_2'D_2$
- The penalty P becomes F (block diagonal matrix):

» Model

### **ANOVA-type Decomposition of Smooth Surfaces:**



<sup>»</sup> Advantage

#### Advantages:

• Extension to *d*-dimensions:

$$B = B_2 \otimes B_1 \otimes \cdots \otimes B_d$$

- Efficient algorithms:
  - Currie et al (2006): Generalized Linear Array Models (GLAM)
- Anisotropy (different smoothing for each dimension):
- Complex models: spatial data smoothing

## **Outline**

1 P-splines

Mixed models approach Multidimensional *P*-splines

2 P-splines for spatial count data

Spatial smoothing
Smooth-CAR model
Application: Scottish L

Application: Scottish Lip Cancer data

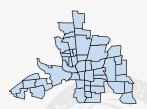
3 Spatio temporal data Smoothing with P-splines ANOVA-Type Interaction Models Application Environmental spatio-temporal data

Spatio-temporal Disease Mapping

# P-splines for spatial count data

P-splines for spatial smoothing

### ▶ We propose:



- 2d P-splines:
- Geostatistics: at sampling locations.
- Regional areal: at the centroids

Models of the form:

- (lon, lat) is a large-scale spatial smooth trend:  $X\beta + Z\alpha$
- The mixed model allows the simultaneous estimation of smoothing and spatial correlation.

# P-splines for spatial count data

P-splines for spatial smoothing

#### ▶ We propose:



- 2d P-splines:
- Geostatistics: at sampling locations.
- Regional/areal: at the centroids.

- Models of the form
  - where
    - (lon, lat) is a large-scale spatial smooth trend:  $X\beta + Z\alpha$
    - The mixed model allows the simultaneous estimation of smoothing and spatial correlation.

P-splines for spatial smoothing

#### ▶ We propose:



- 2d P-splines:
- Geostatistics: at sampling locations.
- Regional/areal: at the centroids.

- Models of the form
- 100
  - C(lon, lat) is a targe-scale spatial smooth trend:  $X\beta + Z\alpha$
  - The mixed model allows the simultaneous estimation of smoothing and spatial correlation.

P-splines for spatial smoothing

#### ▶ We propose:



- 2d P-splines:
- Geostatistics: at sampling locations.
- Regional/areal: at the centroids.

► Models of the form:

$$y = f(lon, lat) + \epsilon$$

- f(lon, lat) is a large-scale spatial smooth trend:  $X\beta + Z\alpha$ .
- The mixed model allows the simultaneous estimation of smoothing and spatial correlation.

<sup>»</sup> Spatial count data

**Basis for Spatial Data** 

- ▶ B-spline Basis for spatial data:
  - Given that data are NOT in an array

$$B = B_2 \otimes B_1$$
 replace by  $B_2 \square B_1$ 

☐ denotes the "Row-wise Kronecker" or **Box-Product**.

#### **Def. Box-Product:**

$$\mathbf{\textit{B}}_{2}\square\mathbf{\textit{B}}_{1}=(\mathbf{\textit{B}}_{2}\otimes\mathbf{1}_{c_{1}})\odot(\mathbf{1}_{c_{2}}\otimes\mathbf{\textit{B}}_{1})$$

 $\odot$  is the "element-wise" product.

- ▶ In many applications:
  - Collect count data observed in regions or areas.
    - E.g.: # of cases of disease or deaths
  - Counts are Poisson distributed.

$$m{y} \sim \mathcal{P}(m{\mu})$$

#### Penalized-GLMM

- *P*-splines as **mixed models**:
  - ► Linear Predictor:

$$\eta = B\theta \Longrightarrow X\beta + Z\alpha$$

► Penalized log-Likelihood:

$$\ell_p(oldsymbol{eta},oldsymbol{lpha};oldsymbol{y}) = \ell(oldsymbol{eta},oldsymbol{lpha};oldsymbol{y}) - rac{1}{2}oldsymbol{lpha}'oldsymbol{F}oldsymbol{lpha}$$

► Estimation via PQL

- ► In many applications:
  - Collect count data observed in regions or areas.
    - E.g.: # of cases of disease or deaths
  - Counts are Poisson distributed.

$$m{y} \sim \mathcal{P}(m{\mu})$$

#### **Penalized-GLMM**

- P-splines as mixed models:
  - ▶ Linear Predictor:

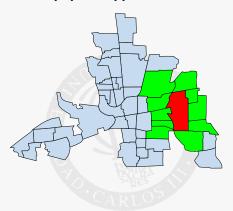
$$\eta = B\theta \Longrightarrow X\beta + \mathbf{Z}\alpha$$

Penalized log-Likelihood:

$$\ell_p(\boldsymbol{eta}, \boldsymbol{lpha}; \boldsymbol{y}) = \ell(\boldsymbol{eta}, \boldsymbol{lpha}; \boldsymbol{y}) - \frac{1}{2} \boldsymbol{lpha}' \boldsymbol{F} \boldsymbol{lpha}'$$

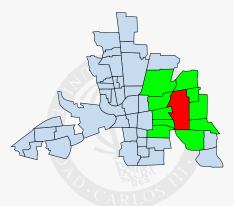
► Estimation via PQL

**CAR** model



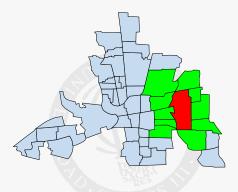
- Conditional Autoregressive Models (CAR), Besag (1991)
  - Spatial Dependence across "neighbours".
- Different neighbourhood criteria.
  - Common border.
  - Centroids distance, 4-nearest neighbours.

**CAR** model



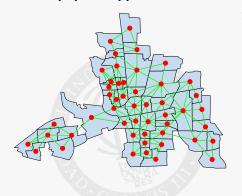
- Conditional Autoregressive Models (CAR), Besag (1991)
- Spatial Dependence across "neighbours".
- Different neighbourhood criteria
  - Common border.
  - Centroids distance, 4-nearest neighbours.

**CAR** model



- Conditional Autoregressive Models (CAR), Besag (1991)
- Spatial Dependence across "neighbours".
- Different neighbourhood criteria.
  - Common border.
  - Centroids distance, 4-nearest neighbours.

**CAR** model



- Conditional Autoregressive Models (CAR), Besag (1991)
- Spatial Dependence across "neighbours".
- Different neighbourhood criteria.
  - Common border.
  - Centroids distance, 4-nearest neighbours.

**CAR model** 

#### ► Formulation:

$$y = X\beta + b$$
,

where  $b = (b_1, b_2, ..., b_n)'$  is a vector for the **spatial effects** 

Impose a spatial dependency structure by a prior distribution for b:

$$oldsymbol{b} \sim \mathcal{N}(oldsymbol{0}, oldsymbol{0})$$

where  $G_b$  depends on the "neighbourhood structure"

defined by Contiguity matrix (Q)

**CAR model** 

#### ▶ Formulation:

$$y = X\beta + b$$

where  $\boldsymbol{b} = (b_1, b_2, ..., b_n)'$  is a vector for the **spatial effects** 

Impose a spatial dependency structure by a prior distribution for b:

$$m{b} \sim \mathcal{N}(m{0}, m{G}_b)$$

where  $G_b$  depends on the "neighbourhood structure":

▶ defined by Contiguity matrix (Q)

**CAR** model

- √ We follow an Empirical Bayes approach:
- ► Intrinsic CAR:

$$G_b = \sigma_b^2 Q^- + \kappa^{-1} I$$

(Besag, 1991)

- Two independent and separate variance components:
  - ▶ Spatially-structured variation:  $\sigma_h^2 Q^-$
  - ▶ Unstructured non-spatial correlation:  $\kappa^{-1}I$
- Alternative CAR models structures

$$= g_b^2 (\phi Q_{LL} + (1 - \phi)I)^{-1}$$

$$\sigma_b^2 \ (\phi \ \Box + (1 - \phi)I)$$
 (Dean et al, 2001)

- $\blacktriangleright$   $\phi$  measures the relative weight between structured and unstructured variability
- $ightharpoonup 0 \le \phi \le 1$

**CAR** model

- √ We follow an Empirical Bayes approach:
- ► Intrinsic CAR:

$$G_b = \sigma_b^2 Q^- + \kappa^{-1} I$$

(Besag, 1991)

- Two independent and separate variance components:
  - ▶ Spatially-structured variation:  $\sigma_b^2 Q^-$
  - ▶ Unstructured non-spatial correlation:  $\kappa^{-1}I$
- ► Alternative CAR models structures:

$$G_b = \sigma_b^2 (\phi Q + (1 - \phi)I)^{-1}$$

(Leroux et al, 1999)

$$G_b = \sigma_b^2 \left( \phi Q^- + (1 - \phi)I \right)$$

(Dean et al, 2001)

- lacktriangledown  $\phi$  measures the relative weight between *structured* and *unstructured* variability
- $ightharpoonup 0 \le \phi \le 1$

Lee and Durban (2009)

- ▶ We propose a "hybrid" model:
  - Spatial P-spline with CAR structure: "Smooth-CAR" model
  - Model:

$$\eta = X\beta + Z\alpha + b ,$$

where  $b \sim \mathcal{N}(\mathbf{0}, G_b)$ 

#### Our approach:

$$\eta =$$
 Spatial Trend

 $X\beta + Z\alpha$ 

(Large-scale)

Local area-level spatial correlation

Spatial Random Effects
(Small-scale)

Lee and Durban (2009)

- ▶ We propose a "hybrid" model:
  - Spatial P-spline with CAR structure: "Smooth-CAR" model
  - Model:

$$\eta = X\beta + Z\alpha + b ,$$

where  $b \sim \mathcal{N}(\mathbf{0}, G_b)$ 

#### Our approach:

$$\eta = \underbrace{ \begin{array}{c} ext{Spatial Trend} \\ ext{} Xeta + Zlpha \end{array}}_{ ext{(Large-scale)}} + \underbrace{ \begin{array}{c} ext{Local area-level spatial correlation} \\ ext{Spatial Random Effects} \\ ext{(Small-scale)} \end{array}$$

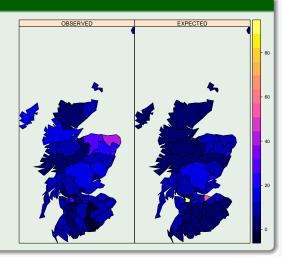
#### **▶** Summary:

Model	Linear Predictor	Area-level var.
Poisson	$Xeta + \mathbf{Z}lpha$	_
CAR	$X\beta + b$	$oldsymbol{b} \sim \mathcal{N}(oldsymbol{0}, oldsymbol{G_b})$
Smooth-CAR	$Xeta + \mathbf{Z}lpha + b$	$oldsymbol{b} \sim \mathcal{N}(oldsymbol{0}, oldsymbol{G_b})$

- ► The Smooth-CAR:
  - lacktriangle Allow us model the **spatial trend** (Xeta+Zlpha) along large geographical distances and
  - ▶ **Local area-level** correlation by a **CAR** component (*b*).

#### **Example: Scottish Lip Cancer**

- Breslow and Clayton (1993)
- Observed (y) and Expected (e) cases of lip cancer
- 56 counties in Scotland
- Period: 1975 1980.



# Fitted Models

#### ▶ We fit several models:

Smooth P-splines models:

$$\eta = \log(e) + X\beta + Z\alpha$$

(Poisson)

log(e) is the **offset** term.

CAR models

$$=\log(a) + X\beta + b$$

$$GI = \sigma_h^2 (\phi O^- + (1 - \phi)I)$$

(Dean

Smooth-CAR models

$$m{y} + m{X}m{eta} + m{Z}m{lpha} + m{b} \;, \quad m{b} \sim \mathcal{N}(m{0}, m{G}_b)$$

# **Application: Scottish Lip Cancer data Fitted Models**

#### ▶ We fit several models:

Smooth P-splines models:

$$\eta = \log(e) + X\beta + Z\alpha$$
 (Poisson)

log(e) is the **offset** term.

CAR models:

$$\eta = \log(e) + X\beta + b, \quad b \sim \mathcal{N}(\mathbf{0}, G_b),$$

with:

$$G_b = \sigma_b^2 \left( \phi Q^- + (1 - \phi) I \right)$$
 (Dean)

Smooth-CAR models

$$(\mathbf{J} + Xoldsymbol{eta} + Zoldsymbol{lpha} + oldsymbol{b} \;, \quad oldsymbol{b} \sim \mathcal{N}(\mathbf{0}, G_b)$$

# **Application: Scottish Lip Cancer data Fitted Models**

#### ▶ We fit several models:

Smooth P-splines models:

$$\eta = \log(e) + X\beta + Z\alpha$$
 (Poisson)

log(e) is the **offset** term.

CAR models:

$$\eta = \log(e) + X\beta + b, \quad b \sim \mathcal{N}(\mathbf{0}, G_b),$$

with:

$$G_b = \sigma_b^2 \left( \phi Q^- + (1 - \phi)I \right)$$
 (Dean)

Smooth-CAR model:

$$\eta = \log(e) + X\beta + Z\alpha + b, \quad b \sim \mathcal{N}(0, G_b)$$

Models comparison criteria

In order to compare the proposed models we use:

$$\begin{aligned} \mathbf{AIC} &= \mathbf{Dev} + 2 \times \mathbf{df} \\ \mathbf{BIC} &= \mathbf{Dev} + \log(n) \times \mathbf{df} \end{aligned}$$

where

df is the effective dimension of the model ("degrees of freedom")

is a measure of the complexity of the fitted model.

$$\hat{y} = H_1$$

Models comparison criteria

In order to compare the proposed models we use:

$$\begin{aligned} \mathbf{AIC} &= \mathbf{Dev} + 2 \times \mathbf{df} \\ \mathbf{BIC} &= \mathbf{Dev} + \log(n) \times \mathbf{df} \end{aligned}$$

- df is the effective dimension of the model ("degrees of freedom").
  - ▶ is a measure of the complexity of the fitted model,
  - ► Calculated as the trace(*H*),

$$\hat{y} = Hy$$

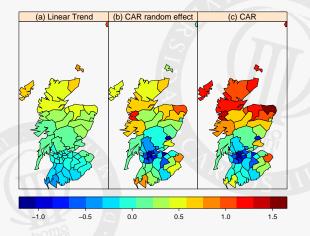
Comparisons of fitted models

			Pai	ameters					
Model		$\lambda_1$	$\lambda_2$	$\sigma_{ m s}^2$	$\kappa^{-1}$	$\phi$	AIC	BIC	df
Smooth:	Poisson	11.75	3.63	-	-	1	114.04	228.46	15.90
CAR:	Dean	-	-	0.78	}	0.99	89.36	179.56	32.78
Smooth-CAR:	Dean	30.11	16.37	0.53	7-	0.97	87.46	175.70	30.64

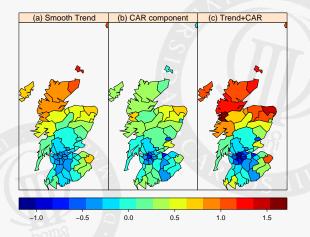
#### ▶ Observations:

- $\phi \approx 1$   $\longrightarrow$  Overdispersion is due to "structured" spatial correlation  $(\sigma_h^2 Q^-)$ .
- Smooth-CAR performs better in terms of the selected criteria.

#### ► Dean's CAR model:



- (a) Large-scale linear trend:  $X\beta$
- (b) CAR structured random effects:  $b \sim \mathcal{N}(\mathbf{0}, G_b)$
- (c)  $X\beta + b$



- (a) Smooth large-scale spatial trend:  $X\beta + Z\alpha$
- (b) CAR structured random effects:  $b \sim \mathcal{N}(\mathbf{0}, G_b)$
- (c)  $X\beta + Z\alpha + b$

### **Outline**

#### 1 P-splines

Mixed models approach Multidimensional *P*-splines

- P-splines for spatial count data
  - Smooth-CAR model
    Application: Scottish Lip Cancer da
- Spatio-temporal data Smoothing with P-splines ANOVA-Type Interaction Models Application Environmental spatio-temporal data
- Spatio-temporal Disease Mapping

# **Spatio-temporal data**

- Response variable,  $y_{ijt}$ 
  - measured over **geographical locations**,  $s = (x_i, x_j)$ , with i, j = 1, ..., n
  - and over time periods,  $x_t$ , for t = 1, ..., T
- ISSUE: huge amount of data available
  - e.g.: Environmental data, epidemiologic studies, disease mapping applications, ...
- Smoothing techniques:
  - Study spatial and temporal trends.
  - Space and time interactions.
  - √ 3-dimensional smoothing: P-splines and GLAM.

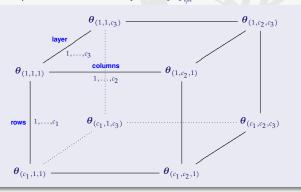
# Example of GLAM in 3d

Currie et. al (2006)

• 3d-case:

$$f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)=\mathbf{B}\boldsymbol{\theta}$$

- Basis:  $B = B_1 \otimes B_2 \otimes B_3$ 
  - $\theta$  can be expressed as a 3d-array  $A = \{\theta\}_{iik}$  of dim.  $c_1 \times c_2 \times c_3$



- 3d-Penalty matrix:
  - Set penalties over the 3*d*-array *A*:

$$P = \lambda_1 \underbrace{D_1'D_1 \otimes I_{c_2} \otimes I_{c_3}}_{ \textbf{row-wise}} + \lambda_2 \underbrace{I_{c_1} \otimes D_2'D_2 \otimes I_{c_3}}_{ \textbf{column-wise}} + \lambda_t \underbrace{I_{c_1} \otimes I_{c_2} \otimes D_t'D_t}_{ \textbf{layer-wise}}$$

For spatio-temporal data:

$$f(\underbrace{\mathsf{longitude}, \mathsf{latitude}}_{\mathbf{Space}}, \mathbf{time})$$

- Spatial anisotropy (λ<sub>1</sub> ≠ λ<sub>2</sub>), different amount of smoothing for latitude and longitude.
- Temporal smoothing  $(\lambda_t)$
- Space-time interaction.

• For spatio-temporal data, we propose:

#### **B-splines Basis:**

$$B = B_s \otimes B_t$$

where

 $\emph{\textbf{B}}_{\emph{s}} \equiv$  is the spatial  $\emph{\textbf{B}}\text{-spline}$  basis  $(\emph{\textbf{B}}_1 \square \ \emph{\textbf{B}}_2)$  and

 $B_t \equiv$  is the *B*-spline basis for time of dim.  $t \times c_3$ .

√ as GLAM:

Given 
$$y_{iit} = Y_{t \times n}$$
, and  $\theta_{ijt} = A_{c_t \times c_s}$ , we have

$$\mathbb{E}[Y] = B_t A B_s'$$

√ as Mixed models

$$B\theta = X\beta + Z\alpha$$

# **Smooth-ANOVA decomposition models**

- Chen (1993), Gu (2002):
  - "Smoothing-Spline ANOVA" (SS-ANOVA).
  - Interpretation as "main effects" and "interactions".
  - Models of type:

$$\widehat{y} = f(x_1) + f(x_2) + f(x_t) 
+ f(x_1, x_2) + f(x_1, x_t) + f(x_2, x_t) 
+ f(x_1, x_2, x_t)$$

"Main/additive effects"

"2-way interactions"

"3-way interactions"

- PROBLEMS:
  - · identifiability, and
  - basis dimension ("curse of dimensionality")

# P-spline ANOVA model for spatio-temporal smoothing

• Lee and Durbán (2009a), consider:

$$y = \gamma + f_s(\mathbf{x}_1, \mathbf{x}_2) + f_s(time) + f_{st}(\mathbf{x}_1, \mathbf{x}_2, time) + \epsilon$$
,

$$f_s(x_1,x_2) \equiv \text{Spatial } 2d \text{ smooth surface} \\ f_t(time) \equiv \text{Smooth time trend} \\ f_{st}(x_1,x_2,time) \equiv \text{Space-time interaction}$$

- We need to construct an identifiable model.
- Our approach is based on:
  - low-rank basis (P-splines)
  - the mixed model representation and SVD properties.

- For each smooth term  $f(\cdot)$ , in spatio-temporal ANOVA model we have
  - B—spline basis:

$$B = [\mathbf{1}_{nt}: B_s \otimes \mathbf{1}_{m{c}} \ \mathbf{1}_n \otimes B_t: m{B}_s \otimes m{B}_t]$$

vector of coefficients

$$oldsymbol{ heta} = (\gamma, oldsymbol{ heta} oldsymbol{ heta}^{(t)'}, oldsymbol{ heta}^{(st)}$$

and a blockdiagonal panalty

- $P_s = 2d$ -spatial penalty
- $P_t = 1d$ -penalty for time
- $P_{st} = 3d$  space-time penalty

- For each smooth term  $f(\cdot)$ , in spatio-temporal ANOVA model we have
  - *B*-spline **basis**:

$$\textbf{\textit{B}} = [\textbf{1}_{nt}: \textbf{\textit{B}}_{s} \otimes \textbf{1}_{t}: \textbf{1}_{n} \otimes \textbf{\textit{B}}_{t}: \textbf{\textit{B}}_{s} \otimes \textbf{\textit{B}}_{t}]$$

vector of coefficients

$$oldsymbol{ heta} = (\gamma, oldsymbol{ heta}) oldsymbol{ heta}^{(t)'}, oldsymbol{ heta}^{(st)}$$

and a blockdiagonal populty

- = 2d-spatial penalty
- $P_t = 1d$ -penalty for time
  - $P_{st} = 3d$  space-time penalty

- For each smooth term  $f(\cdot)$ , in spatio-temporal ANOVA model we have
  - B-spline basis:

$$B = [\mathbf{1}_{nt} : B_s \otimes \mathbf{1}_t : \mathbf{1}_n \otimes B_t : B_s \otimes B_t]$$

vector of coefficients:

$$oldsymbol{ heta} = (\gamma, oldsymbol{ heta}^{(s)'}, oldsymbol{ heta}^{(t)'}, oldsymbol{ heta}^{(st)'})'$$

and a blockdiagonal p nalty

- $P_s = 2d$ -spatial penalt
- $P_t = 1d$ -penalty for time
- $P_{st} = 3d$  space-time penalty

- For each smooth term  $f(\cdot)$ , in spatio-temporal ANOVA model we have
  - B-spline basis:

$$B = [\mathbf{1}_{nt} : B_s \otimes \mathbf{1}_t : \mathbf{1}_n \otimes B_t : B_s \otimes B_t]$$

vector of coefficients:

$$\boldsymbol{ heta} = (\gamma, {oldsymbol{ heta}^{(s)}}', {oldsymbol{ heta}^{(t)}}', {oldsymbol{ heta}^{(st)}}')'$$

• and a blockdiagonal Penalty:

$$oldsymbol{P} = \left( egin{array}{ccc} 0 & & & & & & \ & P_s & & & & \ & & P_t & & & \ & & P_{st} \end{array} 
ight),$$

where

 $egin{array}{ll} P_s &= 2d\mbox{-spatial penalty} \ P_t &= 1d\mbox{-penalty for time} \ P_{st} &= 3d\mbox{ space-time penalty} \end{array}$ 

María Durbán

- However, B is **NOT full column-rank** ("linear dependency")
- Model is **NOT identifiable**

### Solution:

- Reparameterize as a mixed model (using SVD).
- For each term we have:

$$f_s(x_1, x_2) \equiv x_1 : x_2 \qquad (1)$$

$$f_t(x_t) \equiv x_t \qquad (2)$$

$$f_{st}(x_1, x_2, x_t) \equiv x_1 : x_2 : x_t \qquad (3)$$

• Some terms in (1) and (2) also appear in (3).

► The mixed model representation, allow us to identify the columns to remove in order to maintain the identifiability of the model.

and obtain a blockdiagonal penalty F

In P-splines context, this is equivalent to
✓ apply constraints over regression coefficients θ<sub>i,j,k</sub>

- ► For the ANOVA spatio-temporal model, the resultant mixed model reparameterization is equivalent to apply the next constraints:
  - time effect coefficient:

$$\sum_{t=1}^{c_t} \boldsymbol{\theta}_t^{(\mathsf{t})} = 0,$$

 constraints over the spatio-temporal array of coefficients, Θ<sup>(st)</sup>, of dimensions c<sub>t</sub> × c<sub>s</sub>:

$$\sum_{i}^{c_{1}} \boldsymbol{\theta}_{t,ij}^{(\mathrm{st})} = \sum_{j}^{c_{2}} \boldsymbol{\theta}_{t,ij}^{(\mathrm{st})} = \sum_{i}^{c_{1}} \sum_{j}^{c_{2}} \boldsymbol{\theta}_{t,ij}^{(\mathrm{st})} = 0.$$

## In practice

 $\blacktriangleright$  We only need to construct the matrices X, Z and penalty F

$$f_s(x_1,x_2)$$
  $f_t(x_t)$   $f_{st}(x_1,x_2,x_t)$ 

$$egin{array}{llll} X & \equiv & \mbox{by columns} & x_1:x_2 & x_t & (x_1,x_2,x_t) \ & Z & \equiv & \mbox{by blocks} & '' & '' & '' \end{array}$$

$$F \equiv$$
 blockdiagonal  $F_s \qquad F_t \qquad F_{st} \ (\lambda_1, \lambda_2) \qquad \lambda_t \qquad ( au_1, au_2, au_t)$ 

# **Ozone pollution in Europe**

Lee and Durbán (2009a)

- Sample of 45 monitoring stations
- Monthly averages of  $O_3$  levels (in  $\mu g/m^3$  units)
- from january 1999 to december 2005 (t = 1, ..., 84)

### Models:

Additive:

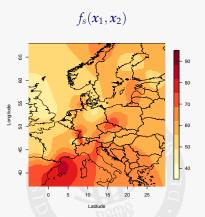
$$f_s(\mathbf{x}_1,\mathbf{x}_2) + f_t(\mathbf{x}_t)$$

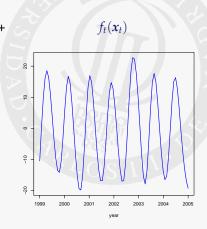
• Spatio-temporal Interaction:

✓ ANOVA:

$$f_s(x_1, x_2) + f_t(x_t) + f_{st}(x_1, x_2, x_t)$$

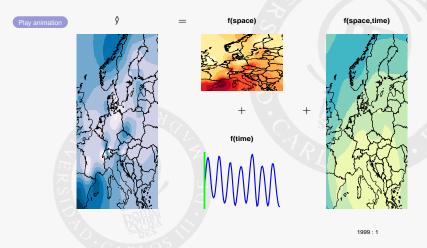
# Spatial 2d + time





- √ Space-time interaction is not considered
- √ time smooth trend is additive

# **Spatio-temporal ANOVA model**

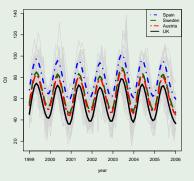


# **Comparison of fitted values**

## Additive VS ANOVA

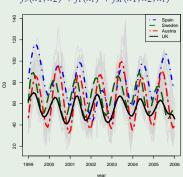
► Additive model fit

$$f_s(x_1, x_2) + f_s(x_t)$$



► ANOVA model fit

$$f_s(x_1,x_2) + f_t(x_t) + f_{st}(x_1,x_2,x_t)$$



- Additive model assumes a spatial smooth surface over all monitoring stations that remains constant over time.
- ✓ ANOVA model captures individual characteristics of the stations throughout time.

# Comparison of Models ANOVA and Additive

Model	AIC	df
ANOVA	14280.73	366.03
Additive	16506.28	65.98

### ▶ Observations:

- Best overall performance of ANOVA in terms of AIC
- ANOVA model is more realistic than Additive, and easier to decompose and interpret in terms of the fit.

## **Outline**

P-splines

Mixed models approach Multidimensional P-splines

P-splines for spatial count data

Spatial smoothing
Smooth-CAR model
Application: Scottish Lip Cancer dat

Spatio temporal data Smoothing with P-splines

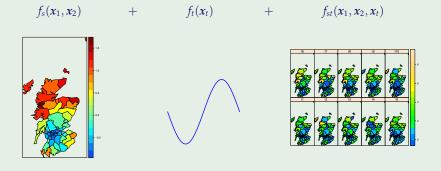
Application Environmental spatio-temporal data

**4** Spatio-temporal Disease Mapping

# **Spatio-temporal Disease Mapping**

## P-spline ANOVA model for disease mapping

- Y and E are t × n arrays of observed and expected cases of disease over t time periods, and M = log(\(\frac{Y}{E}\)).
- Consider an ANOVA model for  $\eta$



## **Summary**

- ▶ New flexible approach for spatial and spatio-temporal data smoothing:
  - based on P-splines as mixed models and
  - ANOVA decomposition
- Methodology also extensible for disease mapping applications.
- Computationally efficient algorithms (GLAM)

## **Bibliography**



Lee, D.-J. and Durbán, M. (2009)

Smooth-CAR mixed models for spatial count data.

Computational Statistics and Data Analysis 53(8):2968-2979.



Lee, D.-J. and Durbán, M. (2009)

*P-spline ANOVA-Type interaction models for spatio-temporal smoothing.*Submitted



Eilers, PHC., Currie, ID. and Durbán, M. (2006)

Fast and compact smoothing on large multidimensional grids.

Computational Statistics and Data Analysis, 50(1):61-76.



Currie, ID., Durbán M. and Eilers, PHC. (2006)

Generalized linear array models with applications to multidimensional smoothing. Journal of the Royal Statistical Society B, 68:1-22.