Considering covariates in the covariance structure of spatio-temporal processes

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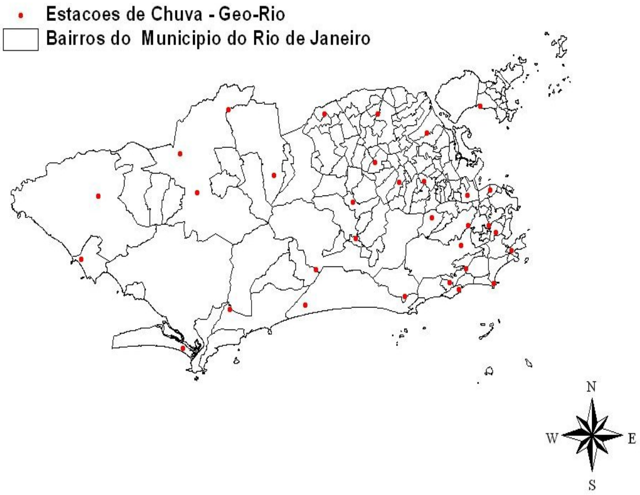
Geostatistics



Rainfall monitoring stations of Rio de Janeiro

Basic Model: Data ($\mathbf{Y}$) are a (partial) realization of a random process (*stochastic process* or *random field*)

$$\{Y(s) : \mathbf{s} \in G\}$$

where G is a fixed subset of $\mathbb{R}^d$ with positive d-dimensional volume. In other words, the spatial index $\mathbf{s}$ varies *continously* throughout the region G.

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GOAL:

- Want a method of predicting $Y(\mathbf{s}_0)$ for any $\mathbf{s}_0$ in G.
- Want this method to be optimal (in some sense).

What do we need?

- Want $Y(\mathbf{s}) : \mathbf{s} \in G$ to be continuous and "smooth enough" (local stationarity)
- description of spatial covariation
- once we obtain the spatial covariation how to get predicted values

Basic Approach: given covariance structure, predict.

Gaussian Processes

Definition:
A function $Y(.)$ taking values $y(s)$ for $s \in G$ has a Gaussian process distribution with mean function $m(.)$ and covariance function $c(.,.)$, denoted by

$$Y(.) \sim GP(m(.), c(.,.))$$

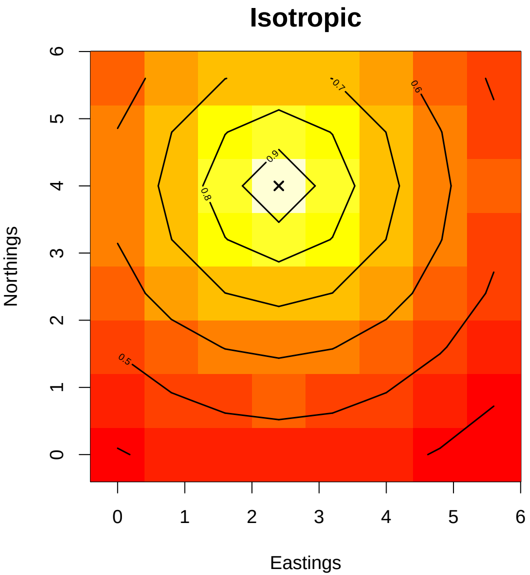
if for any $s_1, \cdots, s_n \in G$, and any $n = 1, 2, \cdots$, the joint distribution of $Y(s_1), \cdots, Y(s_n)$ is multivariate Normal with parameters given by

$E\{Y(s_j)\} = m(s_j)$ and
$Cov(Y(s_i), Y(s_j)) = c(s_i, s_j)$.

Stationarity and isotropy

- In spatial statistics one usually assumes the spatial process to be stationary and isotropic $\rightarrow$ distribution is unchanged when the origin of the index set is translated, and the process is invariant under rotation about the origin
- For any two locations s and s', the spatial correlation is usually modelled as $Corr(Y(s), Y(s')) = c(s, s') = \rho(||s - s'||, \phi)$, where $\rho(.)$ must be a positive definite function $\Rightarrow$ important for spatial interpolations

Visualizing the assumption of isotropy



- In practice, the hypothesis of isotropy is usually violated due to local effects in the correlation structure of the spatial process
- E.g. dispersion of particulate matters, wind speed, ocean temperature, solar radiation, among others

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Modelling anisotropy

Correlation structure could be different in different directions.

Geometrical Anisotropy

It can be corrected by a linear transformation. One possibility is to assume

$$c(s,s') = \rho(\| \, A\,s - A\,s' \, \|), \quad h \in \mathbb{R}^d$$

where A is a unknown $d \times d$ matrix with $\rho(.)$ being a valid correlation function.

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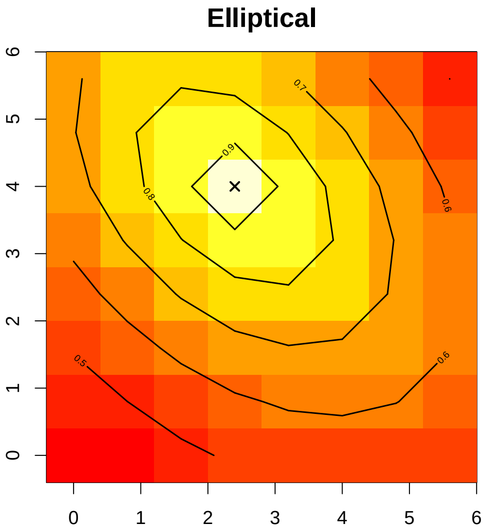


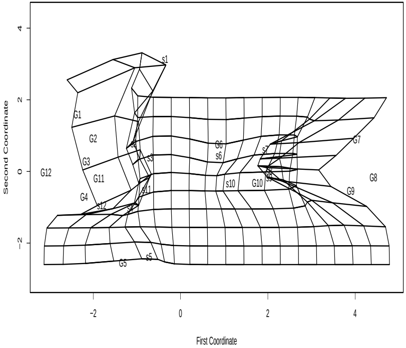
Spatial deformation

- Sampson & Guttorp (JASA, 1992) pioneered an approach to modelling nonstationarity and anisotropy;
- Main idea: nonlinear transformation of the G (Geographical) space, into D space, within which the spatial structure is stationary and isotropic
- In this case, $c(s, s') = \rho(||d(s) - d(s')||)$

Spatial deformation

- Schmidt & O'Hagan (JRSS B, 2003) proposed a Bayesian approach and assigned a GP prior to the mapping function $d(.)$.

The mapping might result in some folding of the original configuration.



Solar radiation dataset (S&G (1992) and S&O (2003)).

Site 1 has a very different altitude when compared to the others.

There are many alternatives to the latent space idea

- Higdon, Swall and Kern (Bayesian Statistics 6 1999)
- Fuentes and Smith (Technical Report NCSU, 2002)
- Fuentes (Biometrika, 2002)
- Kim, Mallick and Holmes (JASA, 2005)
- Paciorek and Shervish (Environmetrics, 2006)

to mention just a few...

All of them make use of highly structured models.

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Using information about covariates to learn about anisotropy

Anisotropy $\Leftrightarrow$ local effects from other variables $\rightarrow$ inclusion of covariates in the covariance structure of the spatial process $\rightarrow$ parsimonious model.

Covariance function must be valid (positive definite)!

Alternatives:

- Schmidt, Guttorp & O'Hagan, *Environmetrics*, 2011
- Reich, Eidvisk, Guindani, Nail & Schmidt, *Annals of Applied Statistics, 2012*
- Vianna Neto, Schmidt & Guttorp (*JRSS, Series C, 2014*)

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Schmidt, Guttorp & O'Hagan (Environmetrics, 2011)

- One way to use covariate information is by allowing the mapping function of Sampson and Guttorp (1992) to be of dimension greater than 2.

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The $\mathbf{d}(.)$ process in $\mathbb{R}^C$

In the general case of D being of dimension $C > 2$, we have that $\mathbf{d}(.) \in R^C$. Following Schmidt (2001)

$$\mathbf{d}(.) \sim GP(\mathbf{m}(.), \boldsymbol{\sigma}_d^2 R_d(.,.)),$$

where

$$\mathbf{R}_d(\mathbf{s}_i, \mathbf{s}_j) = \exp\left\{-(\mathbf{s}_i - \mathbf{s}_j)'\mathbf{B}_d(\mathbf{s}_i - \mathbf{s}_j)\right\},$$

where

- $\mathbf{B}_d$ is a $C \times C$ diagonal matrix with $\mathbf{B}_d = \text{diag}\ (b_d, b_d, b_3, \cdots, b_C)$.
- $\boldsymbol{\sigma}_d^2 = \text{diag}\ (\sigma_{d_{11}}^2, \sigma_{d_{22}}^2, \cdots, \sigma_{d_{CC}}^2)$
- Possibilities for the mean include: $\mathbf{m}_i = (lat_i, long_i, 0, \cdots, 0)'$ or $\mathbf{m}_i = (lat_i, long_i, stalt_i, stcov_1, \cdots, stcov_{C-2})'$

A deterministic mapping

Define

$$d(\mathbf{s},\mathbf{s}') = \sqrt{(\mathbf{s}-\mathbf{s}')^T\,\Phi^{-1}\,(\mathbf{s}-\mathbf{s}')}, \tag{1}$$

as the Mahalanobis distance between $\mathbf{s}$ and $\mathbf{s}'$, which is a function of the arbitrary positive definite matrix Φ. A valid covariance function might assume, e.g.

$$S(\mathbf{s},\mathbf{s}';\Phi,\sigma^2) = \sigma^2 \exp\left(-d(\mathbf{s},\mathbf{s}')\right). \tag{2}$$

Notice that we can rewrite equation (1) as

$$d(\mathbf{s},\mathbf{s}') = \sqrt{(\mathbf{d}(\mathbf{s})-\mathbf{d}(\mathbf{s}'))^T(\mathbf{d}(\mathbf{s})-\mathbf{d}(\mathbf{s}'))}, \tag{3}$$

where $\mathbf{d}(\mathbf{s}) = \mathbf{A}\mathbf{s}$, and $\Phi = \mathbf{A}^T\mathbf{A}$.
This can be seen as a transformation of the original $\mathbb{R}^2$ space made through the use of covariates.

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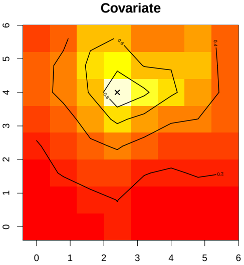
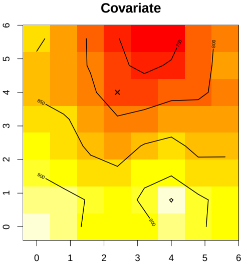
Example of a covariate dependent correlation structure





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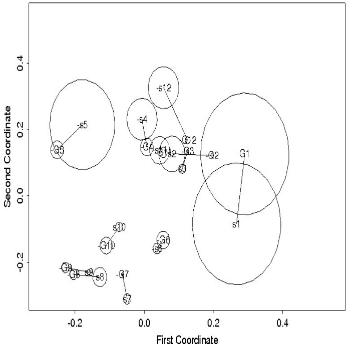
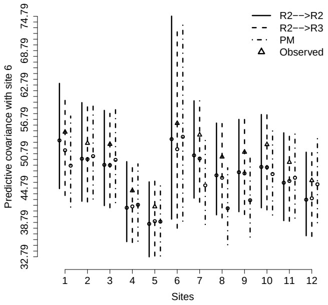
Revisiting the solar radiation dataset

(Schmidt, Guttorp & O'Hagan, Environmetrics, 2011)





Reich, Eidvisk, Guindani, Nail and Schmidt, *Annals of Applied Statistics, 2011*

- Allow for covariate effects when modelling ozone levels in the East coast of the US

$$S(s,t) = \sum_{j=1}^{M} w_j[\mathbf{x}(s,t)]\theta_j(s,t)$$

where

$$w_j[\mathbf{x}(s,t)]^2 = \frac{\exp(\mathbf{x}(s,t)^T\alpha_j)}{\sum_{l=1}^{M}\exp(\mathbf{x}(s,t)^T\alpha_l)}$$

and

$$\theta_j(s,t) = \gamma_j\theta_j(s,t-1) + e_j(s,t) \quad e_{jt} \sim GP(0,K_j)$$

$\mathbf{x}(s,t)$=(mean temperature, max. temp., wind speed, cloud cover)

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Accounting for spatially varying directional effects in spatial covariance structures

J.H. Vianna Neto, A. M. Schmidt and P. Guttorp

JRSS, Series C, 2014, 63, 1, 102-122

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Motivation

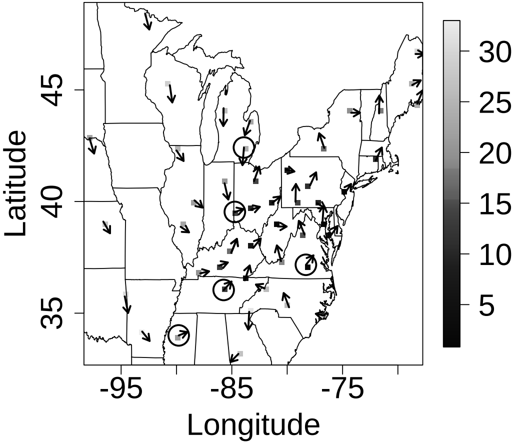

Figure : Observed values of ozone (solid squares in grayscale), and respective wind direction (arrows) for December, 11th, 2008, 3pm.

Process convolution

A stochastic process can be constructed by convolving a latent process $W(\cdot)$ with a smoothing kernel $k(\cdot)$, i.e.,

$$S(s) = \int_G k\,(s-h)\,W\,(h)\,dh. \tag{4}$$

Higdon et al. (1999) propose a Gaussian kernel such that

$$k(s, s-h) = (2\pi)^{-1} \mid \Sigma\,(s) \mid^{-0.5} \exp\left\{-\frac{1}{2}(s-h)^T\Sigma(s)^{-1}(s-h)\right\}.$$

$\Sigma(s)$ is modelled through the connection between a bivariate normal distribution and its one standard deviation ellipse.

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- Paciorek and Shervish (2006) generalize the kernel convolution approach.
  They obtain a nonstationary version of the Matérn covariance function,

$$C(s_i, s_j) = \sigma^2 \frac{1}{\Gamma(\nu) 2^{\nu-1}} |\Sigma(s_i)|^{-1/4} |\Sigma(s_j)|^{-1/4} \left| \frac{\Sigma(s_i)+\Sigma(s_j)}{2} \right|^{-1/2} \left(2\sqrt{\nu Q_{ij}}\right)^{\nu} \kappa_\nu \left(2\sqrt{\nu Q_{ij}}\right),$$

  where $Q_{ij} = (s_i - s_j)^T \left(\frac{\Sigma(s_i)+\Sigma(s_j)}{2} \right)^{-1} (s_i - s_j)$, $\nu > 0$ is the shape parameter, and $\kappa_\nu(.)$ is the modified Bessel function of the second kind of order ν.
- They propose to model $\Sigma(s_i) = \Gamma_i \Lambda_i \Gamma_i^T$, where Λ_i is a diagonal matrix of eigenvalues, $\lambda_1(s_i)$ and $\lambda_2(s_i)$, and Γ_i is an eigenvector matrix.

A covariate dependent kernel (LGA)

Following Higdon

$$S(s) = \int_G k_{s,x}(h)W(h)dh, \text{ for } s, h \in G \subset \mathbb{R}^2, \qquad (5)$$

Let $x(s) = (u(s), v(s))'$ be a directional covariate observed at location s, we first propose

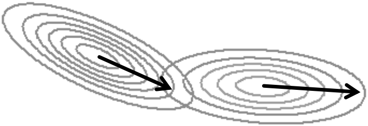
$$\Sigma(s,x) = \Gamma(s,x)^T \Lambda \Gamma(s,x)$$

$$\text{where } \Gamma(s,x)^T = \begin{bmatrix} \cos\,\omega(x(s)) & -\sin\,\omega(x(s)) \\ \sin\,\omega(x(s)) & \cos\,\omega(x(s)) \end{bmatrix}$$

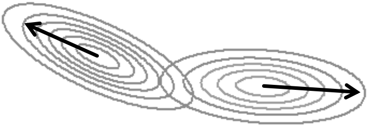
$$\text{and } \Lambda = \begin{bmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{bmatrix},$$

and $\omega(x(s)) = \arctan\left(\frac{v(s)}{u(s)}\right)$.

Drawback of the locally Geometric Anisotropic model



(a) Wind vectors blowing at the same direction



(b) Wind vector blowing at opposite directions

Figure : Illustration of the contours of the kernel matrix based on locations with contrasting wind information (black arrows).

Non-Gaussian kernel based on a projection

Projection of the mean direction as a measure of alignment

Let $x(s)$ represent the directional information at location $s \in G$, with $||x(s)|| = 1$. Now, let

$$r(x(s), x(s^*)) = (x(s) + x(s^*))/2$$

be the mean vector considering locations s and s^* in G.

The projection of the mean vector over the set $\{b \times (s - s^*) + s^* : b \in \mathbb{R}\}$ (straight line that passes through s and s^*) is

$$proj_x(s, s^*) = \frac{\langle r\left(x(s), x(s^*)\right), (s - s^*)\rangle}{\langle (s - s^*), (s - s^*)\rangle} \times (s - s^*).$$

We consider $||proj_x(s, s^*)||$.

Illustration

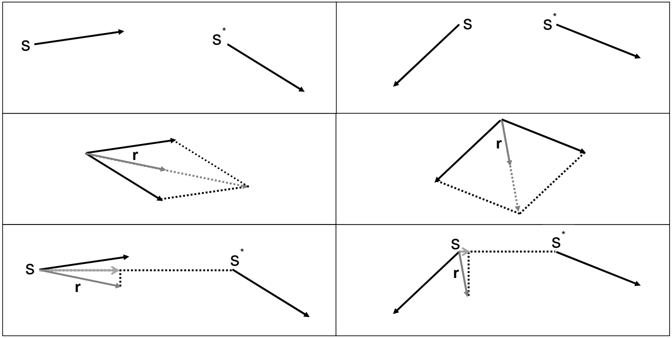


Figure : Diagram with directions (black arrows), mean direction (r) and projection (gray arrows).

The bigger (smaller) the angle between the mean vector and the direction between the two locations, the smaller (bigger) is $||proj_x(s, s^*)||$.

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Modelling $k_{s,x}(.)$

Here, the kernel function is modelled as

$$k_{s,x}(h) = \frac{\sigma \alpha_{s,x}(h)}{\sqrt{\int_G \alpha_{s,x}(h)^2 \, dh}}, \tag{6}$$

We assume

$$\alpha_{s,x}(h) = \begin{cases} \exp\left(-\frac{\|s-h\|}{\phi_1 + \phi_2 \|proj_x(h)\|}\right), & \text{if } s \neq h \\ 1, & \text{if } s = h. \end{cases} \tag{7}$$

Here $H = \{h_1, \cdots, h_m\}$ is a regular grid of points in G. We denote this as the projection model.

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How does this process behave?

Joaquim has written `R-TclTk` softwares that produce graphical correlations, covariances and simulations from the proposed models for different values of the parameters.

Model

We assume

$$Y(s) = \mu(s) + S(s) + \epsilon(s), \; \epsilon(s) \sim N(0, \tau^2),$$

- $\mu(s) = W(s)\,\beta$, $W(s)$ vector of possible covariates
- $S(.)$ and $\epsilon(.)$ are independent
- τ^2 is nugget effect

Inference Procedure

Let $\mathbf{y} = (y(s_1), \cdots, y(s_n))'$ be a partial realization from a Gaussian process with mean vector $\boldsymbol{\mu}$ and covariance matrix Σ, the likelihood function is given by

$$L(\mathbf{y}; \boldsymbol{\theta}) = (2\pi)^{-n/2} \mid \Sigma \mid^{-1/2} \exp\left\{ -\frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right\}.$$

where $\Sigma = \tau^2 (I_n + \eta^{-1}\, \Omega(\boldsymbol{\delta}))$, and $\eta = \tau^2/\sigma^2$,
$\boldsymbol{\delta} = (\delta_1, \delta_2, \cdots, \delta_k)$ be the parameter vector of the kernel function, and
$\Omega(\boldsymbol{\delta})$ is the associated resultant covariance matrix.

The parameter vector to be estimated is $\boldsymbol{\theta} = (\boldsymbol{\mu}, \tau^2, \eta, \boldsymbol{\delta})$.

Bayesian paradigm $\Rightarrow$ MCMC to obtain samples from the resultant posterior distribution.

Ozone levels in the Eastern USA

Measurements of ozone observed at 3pm, on November, 11th, 2008.

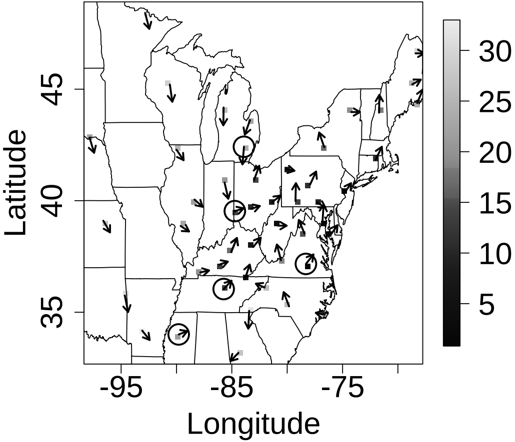

Figure : Observed values of ozone (solid squares in grayscale), and respective wind direction (arrows) for December, 11th,

Ozone levels in the eastern USA

M1 Isotropic model with Matérn covariance function

M2 Elliptical anisotropic model with Matérn covariance function, that is

$$Cov(Y(s_i), Y(s_j)) = \sigma^2 \left(2^{\nu-1}\Gamma(\nu)\right)^{-1} \left(\frac{\sqrt{\|u\|^T \Lambda \|u\|}}{\varphi}\right)^{\nu} \kappa_\nu \left(\frac{\sqrt{\|u\|^T \Lambda \|u\|}}{\varphi}\right)$$

where

$$\Lambda = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix},$$

M3 Nonstationary Matérn covariance function with $\Sigma(s, x)$

M4 Covariance function based on the Projection model

M5 Nonstationary Matérn covariance function with $\Sigma(s)$ as in Paciorek and Shervish (2006)

Results - Computational Time

Model	Computational time	No. Iterations minute
M1	7 min	7142.85
M2	1 h 26 min	581.39
M3	1 h 55 min	434.78
M4	21 min	2380.95
M5	144 h 30 min	80.73

Table : Computational time, and number of iterations per minute, to run the MCMC algorithm for 50,000 iterations for models M1, M2, M3, M4, and 700,000 iterations for model M5 in an Intel(R) Core(TM)2 Quad CPU Q9550 2.83GHz computer with 4 GB of RAM.

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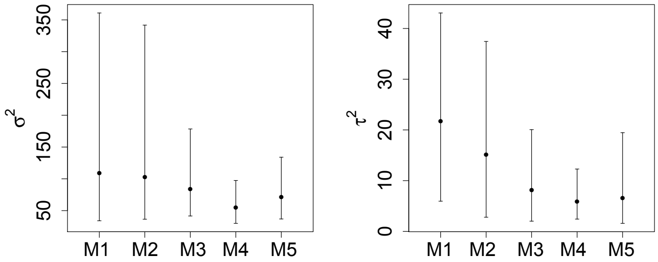
Results - Model comparison

Model	PPL			DIC			Predictive likelihood
	G	P	D_1	$\overline{D}$	p_D	DIC	
M1	458.77	1395.79	1625.18	326.06	3.04	329.10	2.33×10^{-08}
M2	251.37	1050.26	1175.95	318.70	-1.80	316.37	6.18×10^{-08}
M3	87.80	639.06	682.96	309.46	3.88	313.34	6.49×10^{-07}
M4	90.38	464.93	510.12	289.79	4.03	293.82	4.93×10^{-06}
M5	59.97	539.60	569.59	302.29	3.03	305.32	9.98×10^{-08}

Table : Model comparison criteria: PPL, DIC, the predictive likelihood (based on the circled locations) under each fitted model.

Results - Posterior summary of hyperparameters



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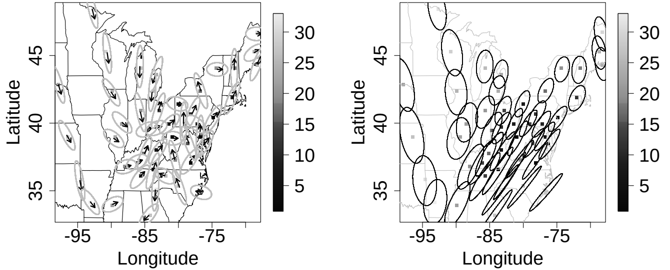
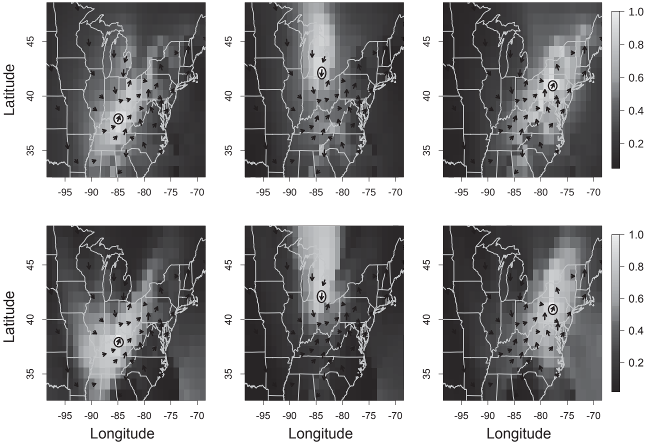
Results - Posterior mean of ellipses under M3 and M5

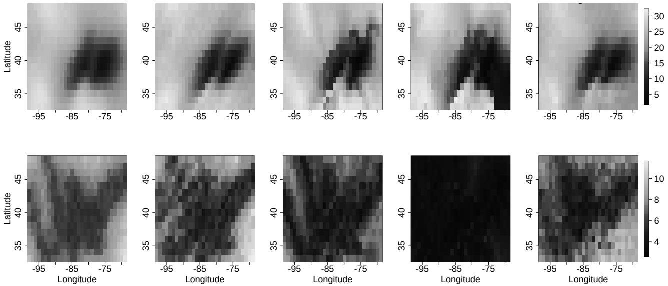


(c) Estimated ellipses under M3 (d) Estimated ellipses under M5

Results - Correlation between a point and all the others

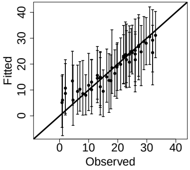


Results - Spatial interpolation

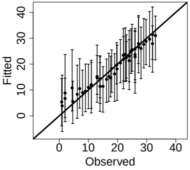


(a) M1 (b) M2 (c) M3 (d) M4 (e) M5

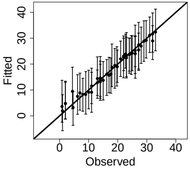
Results - Fitted values



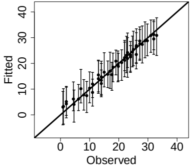
(f) M1



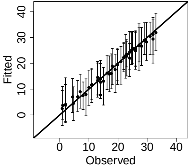
(g) M2



(h) M3



(i) M4



(j) M5

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Discussion

- We propose two different ways of considering directional information in the covariance structure of a spatial process
- This is done by including the covariate in the kernel function of Higdon's and co-authors approach
- Use of the directional covariate significantly reduces the number of parameters in the model while still allowing for some flexibility in the resultant covariance structure.
- Introducing covariates in the covariance structure of spatial processes might be a helpful tool for understanding sources of anisotropy

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