

Spatial temporal modeling, estimation and prediction of environmental processes

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Constructing maps of pollution levels is vital for air quality management, and presents statistical problems typical of many environmental applications. Ideally, such maps would be based on a dense network of monitoring stations, but this does not often exist.

Instead, there are usually two sources of information about pollution levels in the U.S.; sparse sites from monitoring networks, and the output of air quality numerical models.

Combining both sources of information should lead to improved spatial-temporal estimation and prediction.

THE PROBLEM: Misalignment

- **Air quality models output are averages over $36\text{km} \times 36\text{km}$ grid squares, while the observations are at points in space; the two are thus not directly comparable (change of support problem).**
- **For air pollution mapping we need meteorological covariates. Generally, the weather stations are at different locations than the monitoring sites (spatial misalignment).**
- **Any statistical modeling is challenging due to the lack of stationarity, separability and sparseness of the monitoring sites.**

THE SOLUTION: We develop an approach to produce maps that combine model predictions with observations in a coherent way. Combining both sources of information, versus using just the sparse data field or the unreliable model output, should lead to improved estimation of air quality.

Basic idea: We specify a simple model for both numerical models predictions and field data in terms of the unobserved ground truth, and estimate it in a Bayesian way.

Our approach takes account of and estimates the bias in the models, the lack of stationarity, and separability in the data, the change of support problem, and the uncertainty about these factors.

Environmental applications

Two sources of information for air pollutants:

- **Monitoring data**
- **Numerical models**

In the next 2 applications, we seek to combine monitoring data with numerical model output to improve the spatial-temporal estimation and prediction.

Environmental applications

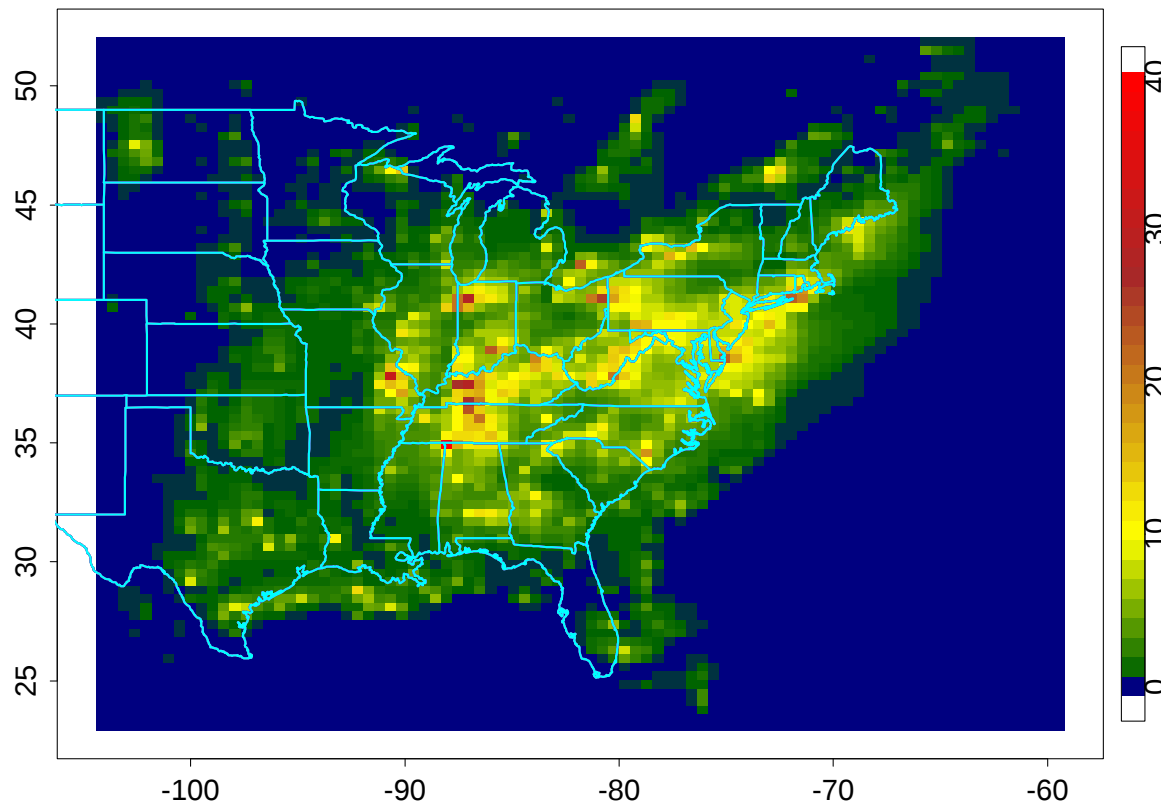
Regional Models (Models-3) Estimated Concentrations and fluxes

The present generation of regional scale air quality models considers land cover, plant growth rate, topography, and other factors in estimating pollutant concentrations and deposition fluxes in a regular grid. The current resolution of the models is $36 \text{ km} \times 36 \text{ km}$. The outputs of Models-3 are not point measurements but hourly areal estimations of the average concentrations and fluxes of different pollutants for each grid cell of $36 \text{ km} \times 36 \text{ km}$.

Models-3 produces estimates of most pollutants, including: Particulate Matter (example 1).

Environmental applications

SO₂ Concentrations



Output of
Models-3, weekly average of SO_2 concentrations (ppb), for
the week of July 11, 1995. The resolution is $36\text{km} \times 36\text{km}$.

Environmental applications

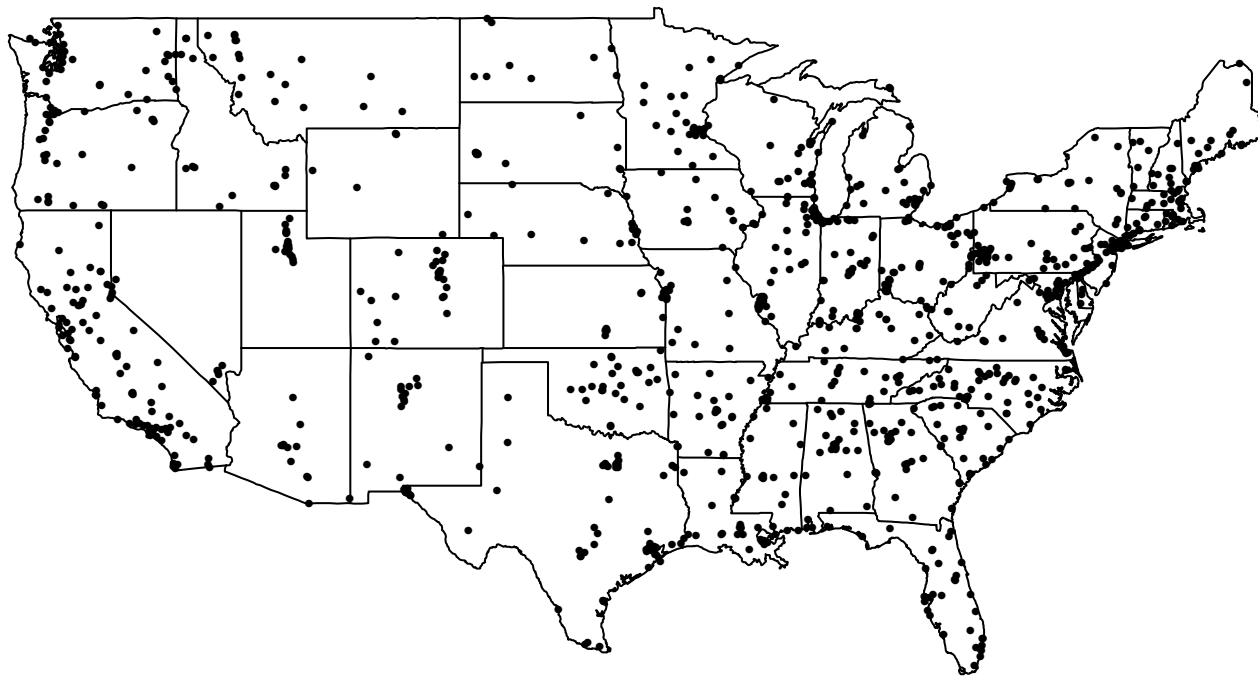
Example 1: concentrations of Particulate Matter

There are two main monitoring networks for ambient PM_{2.5} in the U.S.

- The Federal Reference Method (FRM) monitoring network. Following the guidance on monitoring published by EPA, a national network of about 1000 PM_{2.5} monitoring sites has been established (with PM measurements every 3 or 4 days).
- The Interagency Monitoring of Protected Visual Environments (IMPROVE) network program includes measurement of the composition and concentration of the fine particles at 156 national parks and wilderness areas as required by the Clean Air Act.

Environmental applications

FRM monitoring network



Environmental applications



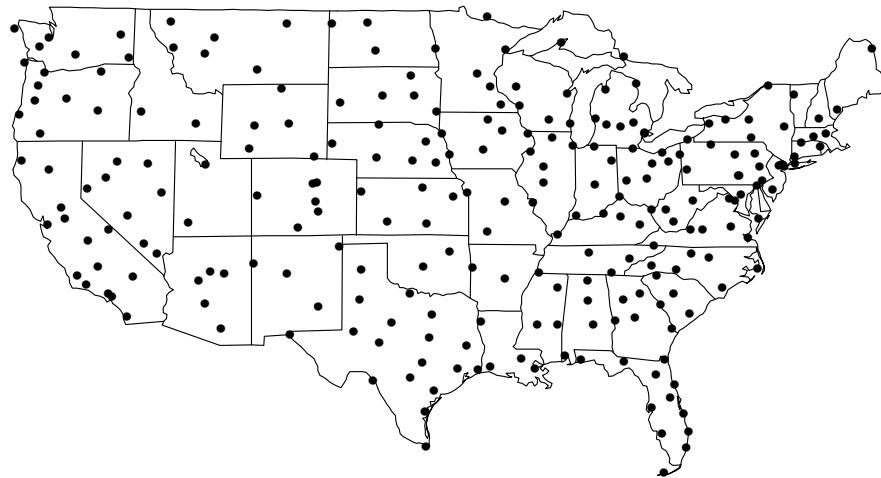
Interagency Monitoring of Protected Visual Environments Program (IMPROVE) Monitoring Sites in the Conterminous U.S. & Virgin Islands.

Environmental applications

Meteorological Covariates

Weather stations with climatic data (daily max. temperature, specific humidity, wind) for 272 sites across the whole US.

met25 Locations



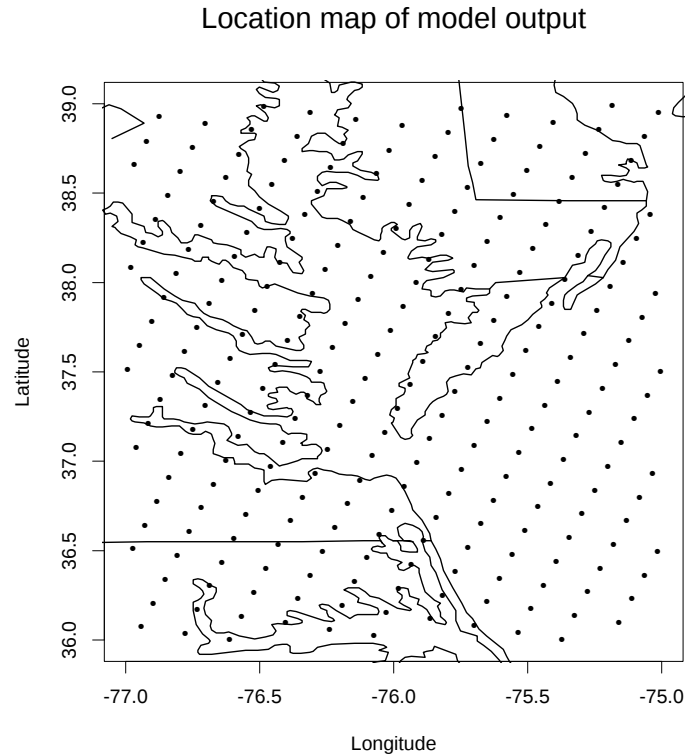
Environmental applications

Example 2: Wind fields

Area of study: The Chesapeake Bay (US). Variable of interest: wind speed. July 2002 (daily forced winds).



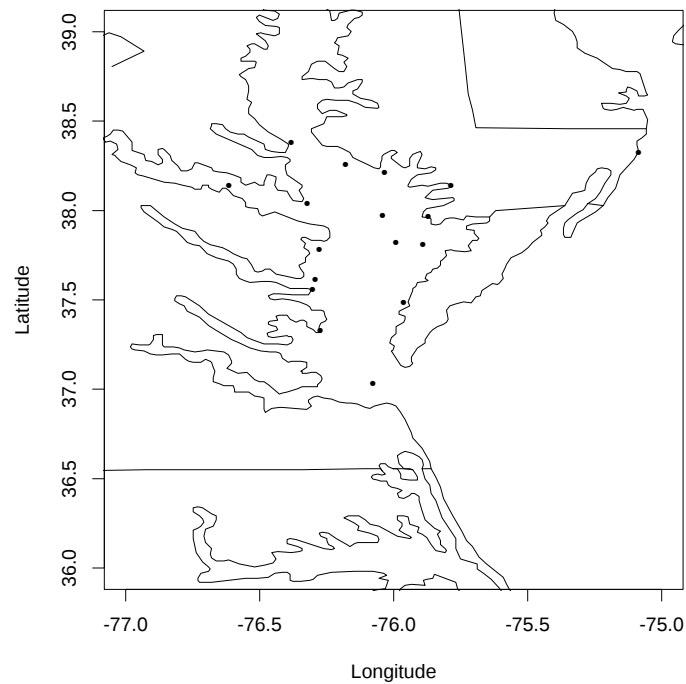
Environmental applications



Grid for the output of a weather prediction numerical model (MM5) in the Chesapeake Bay (US). We have data every 1/2 hour with 15km spatial resolution. We use MM5 36 hours forecast.

Environmental applications

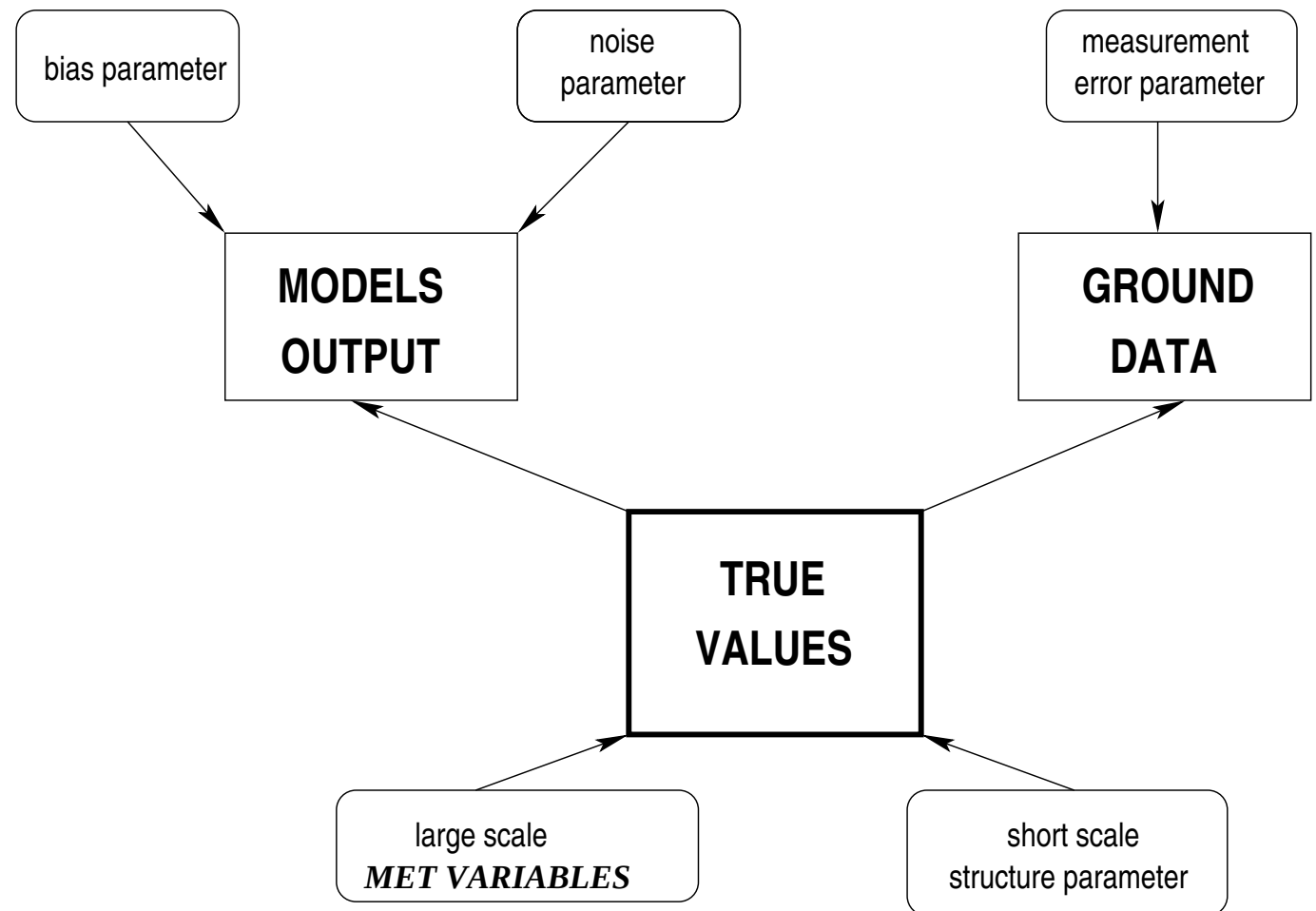
Location map of monitoring sites



Location of the monitoring stations (hourly measurements).

Hierarchical Bayesian melding

Statistical framework (Fuentes and Raftery, 2005, *Biometrics*)



Hierarchical Bayesian melding

MONITORING DATA:

We should not treat **monitoring data** ($\hat{Z}$) as the "ground truth". We assume there is some smooth **underlying** (but unobserved) field $Z(s, t)$, where $Z(s, t)$ measures the "true" concentration of the pollutant at location s and time t . We write

$$\hat{Z}(s, t) = Z(s, t) + e(s, t)$$

where $e(s, t) \sim N(0, \sigma_e^2)$ represents the measurement error (nugget) at location s .

Hierarchical Bayesian melding

Since the output of **Models-3** ($\tilde{Z}$) are not point measurements but areal estimations in subregions $B_1, \dots, B_N$ that cover the domain, D , we have:

$$\tilde{Z}(B_1, t) = a(B_1, t) + b \int_{B_1} Z(\mathbf{s}, t) d\mathbf{s} + \delta(B_1, t)$$

$a(\mathbf{s}, t)$ measures the **additive bias** of the air quality models at location $\mathbf{s}$ and time t , and the parameter function b accounts for the **multiplicative bias** in the air quality models. The process $\delta(\mathbf{s}, t) \sim N(0, \sigma_\delta^2)$ explains the random deviation at location $\mathbf{s}$ with respect to the underlying true process $Z(\mathbf{s}, t)$.

Hierarchical Bayesian melding

The true underlying process Z is a nonstationary spatial process,

$$Z(s, t) = \mu(s, t) + \epsilon(s, t)$$

where $Z(s, t)$ has a spatial-temporal large scale trend, $\mu(s, t)$, that is a function of some **meteorological** covariates $f_1, \dots, f_p$, with unknown coefficients β :

$$\mu(s, t) = \sum \beta_i(s, t) f_i(s, t)$$

The coefficients β vary on space and time.

We assume $Z(s, t)$ has zero-mean uncorrelated errors $\epsilon(s, t)$.

Hierarchical Bayesian melding

The covariates coefficients β , can be modeled using a simple **dynamic spatiotemporal model** with a purely temporal component, γ_t , and a spatiotemporal component $\gamma(\mathbf{s}, t)$:

$$\beta(\mathbf{s}, t) = \gamma_t + \gamma(\mathbf{s}, t)$$

with

$$\gamma(\mathbf{s}, t) = \gamma(\mathbf{s}, t - 1) + \eta(\mathbf{s}, t)$$

η is a spatial-temporal correlated error term.

Hierarchical Bayesian melding

Two particular cases:

- In some cases we might not have covariates. Then, we write $f_i(s, t) = 1$, this means the large scale trend of Z is modeled using the dynamic space-time modeled previously described.
- In other cases the covariates might be unknown at some locations or times, then we model the covariates using the previous space-time dynamic model and input their values in one of the stages of our hierarchical model.

Hierarchical Bayesian melding

The error process $\eta(s, t)$ might have a **nonstationary and nonseparable covariance** with parameter vector θ that might change with location and time.

Air Quality mapping

- Air Quality mapping by combining observations and numerical model output

If the goal is to get more reliable maps of air pollution, we could predict the value of Z (the truth) at location $\mathbf{x}_0$ and time t given ALL the data (monitoring data and Models-3), thus we need the predictive distribution of $Z(\mathbf{x}_0, t)$ given the observations ($\hat{Z}$ and $\tilde{Z}$).

For spatial prediction we simulate values of Z from the posterior predictive distribution:

$$P(Z|\hat{Z}, \tilde{Z}).$$

Validation of numerical models

- **Evaluation of MODELS-3:**

For model evaluation we simulate values of the observed process $\hat{Z}$ given models-3, from the following posterior predictive distribution:

$$P(\hat{Z}|\tilde{Z}, a = 0, b = 1).$$

Validation of numerical models

- **Evaluation of MODELS-3:**

For model evaluation we simulate values of the observed process $\hat{Z}$ given models-3, from the following posterior predictive distribution:

$$P(\hat{Z}|\tilde{Z}, a = 0, b = 1).$$

- **Estimating Bias of Models-3:**

For bias removal we simulate values of the parameters a and b from the posterior distribution:

$$P(a, b|\hat{Z}, \tilde{Z}).$$

We propose the following Gibbs sampling approach for the Bayesian melding method,

Stage 1. We sample from the conditional posterior of the parameters (β, θ) , that represent the lack of stationarity of Z .

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Stage 1. We sample from the conditional posterior of the parameters (β, θ) , that represent the lack of stationarity of Z .

Stage 2. We sample from the conditional posterior distribution of the parameters that explain the bias of $\tilde{Z}$ and the measurement error of $\hat{Z}$ and $\tilde{Z}$, namely $(\sigma_e^2, a, b, \sigma_\delta^2)$.

Gibbs sampling

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Stage 2. We sample from the conditional posterior distribution of the parameters that explain the bias of $\tilde{Z}$ and the measurement error of $\hat{Z}$ and $\tilde{Z}$, namely $(\sigma_e^2, a, b, \sigma_\delta^2)$.

Stage 3. We simulate values of Z the unobserved true values (and the covariates) at the locations where we have measurements from the process $\hat{Z}$ and $\tilde{Z}$.

Nonseparable and nonstationary models

Many of the problems of space and time modeling can be overcome by using separable processes.

A spatial-temporal field $Z(s, t)$, where s represent space and t time, is separable if

$$\text{Cov}\{Z(s, t), Z(s', t')\} = C_1(s, s')C_2(t, t')$$

for some spatial autocorrelation C_1 and temporal autocorrelation C_2 .

Nonseparable and nonstationary models

A class of nonseparable spatial-temporal models have been proposed by Cressie and Huang (JASA, 99), Gneiting (JASA, 02), and by Stein (2003).

Fuentes, (2002c), Fuentes et al. (2004)

Here we define a new class of generalized spectral representations for **nonstationary and nonseparable** spatial temporal processes. For this new class of spatial temporal models the spectral representation itself and the corresponding spectral distribution function (or spectral density) can change slowly on space and time.

Nonseparable and nonstationary models

Background. If Z is a stationary process with autocovariance C , then we can represent the process in the form of the following Fourier-Stieltjes integral:

$$Z(\mathbf{s}) = \int_{\mathbb{R}^2} e^{i\boldsymbol{\omega}^T \mathbf{s}} dY(\boldsymbol{\omega})$$

$Y(\boldsymbol{\omega})$ is called the **spectral process** associated to Z . We define

$$f(\boldsymbol{\omega}) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \exp(-i\boldsymbol{\omega}^T \mathbf{x}) C(\mathbf{x}) d\mathbf{x}$$

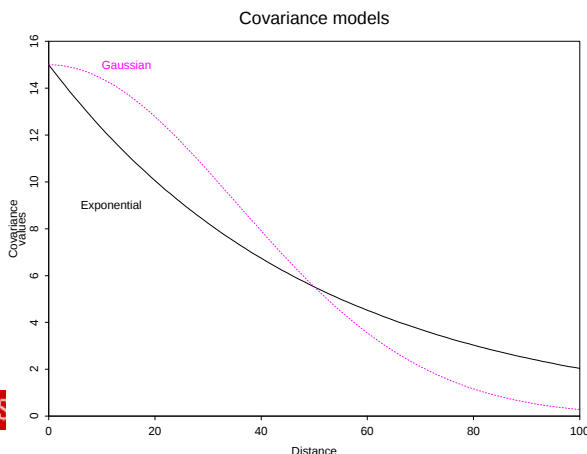
f is the **spectral density**. *Reference Books: Yaglom, 1987; Stein, 1999.*

Nonseparable and nonstationary models

Matérn spectral density, (Matérn, 1986)

$$f(\omega) = \phi(\alpha^2 + |\omega|^2)^{(-\nu)}$$

Here, the vector of covariance parameters is $\theta = (\phi, \nu, \alpha)$. The parameter α^{-1} can be interpreted as the autocorrelation range; $\nu > d/2$ measures the degree of smoothness of Z , and ϕ is a scale parameter.



Nonseparable and nonstationary models

Let Z be a nonseparable process, we propose the following representation

$$Z(\mathbf{x}, t) = \int_{\mathbb{R}^3} \exp(i\mathbf{x}^T \boldsymbol{\omega} + it\tau) \phi_{\mathbf{x}, t}(\boldsymbol{\omega}, \tau) dY(\boldsymbol{\omega}, \tau).$$

It is easy to see that then the covariance function, C , of the nonseparable process $Z(\mathbf{x}, t)$ is given by the formula

$$\begin{aligned} \text{cov}\{Z(\mathbf{x}_1, t_1), Z(\mathbf{x}_2, t_2)\} &= C(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \\ &\int_{\mathbb{R}^3} \mathbf{e}^{i(\mathbf{x}_1 - \mathbf{x}_2)^T \boldsymbol{\omega}} \mathbf{e}^{i(t_1 - t_2)^T \tau} \phi_{\mathbf{x}_1, t_1}(\boldsymbol{\omega}, \tau) \phi_{\mathbf{x}_2, t_2}^c(\boldsymbol{\omega}, \tau) d\boldsymbol{\omega} d\tau \end{aligned} \quad (1)$$

Nonseparable and nonstationary models

In particular

$$\text{var}\{Z(\mathbf{x}, t)\} = C(\mathbf{x}, t; \mathbf{x}, t) = \int_{\mathbb{R}^2} |\phi_{\mathbf{x},t}(\boldsymbol{\omega}, \tau)|^2 d\boldsymbol{\omega} d\tau$$

The spectral density f of Z changes with space and time to explain how the spatial temporal dependency varies on the domain of interest:

$$f_{\mathbf{x},t}(\boldsymbol{\omega}, \tau) = |\phi_{\mathbf{x},t}(\boldsymbol{\omega}, \tau)|^2$$

Nonseparable and nonstationary models

Locally (in a neighborhood of $s_i = (\mathbf{x}_i, t_i)$) we propose the following parametric model for f ,

$$f_{s_i}(\boldsymbol{\omega}, \tau) = \gamma_i (\alpha_i^2 \beta_i^2 + \beta_i^2 |\boldsymbol{\omega}|^2 + \alpha_i^2 |\tau|^2 + \epsilon |\boldsymbol{\omega}|^2 \tau^2)^{-\nu_i}, \quad (2)$$

where γ_i , α_i and β_i are positive, $\nu_i > \frac{d+1}{2}$ and $\epsilon \in [0, 1]$. The parameter α_i^{-1} explains the rate of decay of the spatial correlation. For the temporal correlation, the rate of decay is explained by the parameter β_i^{-1} , γ_i is a scale parameter.

Nonseparable and nonstationary models

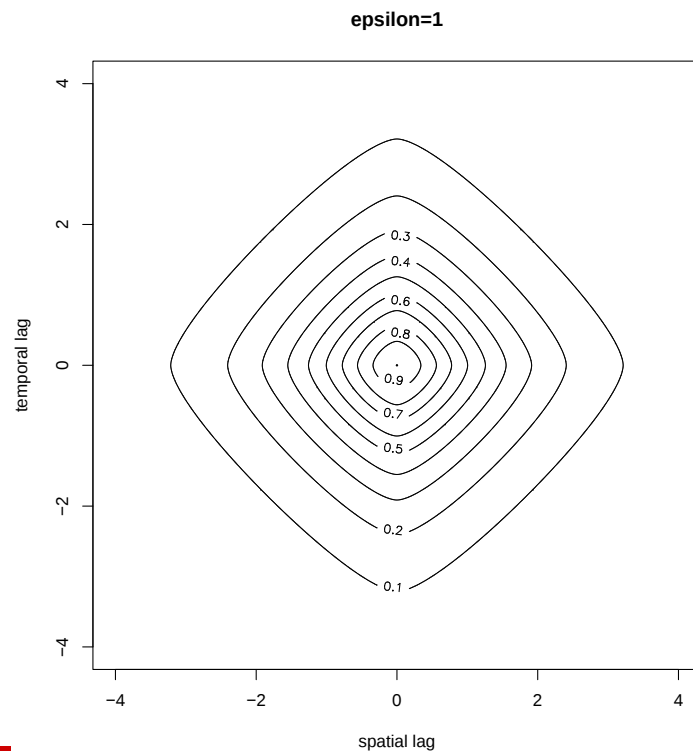
When $\epsilon = 1$, the previous equation can be written as

$$\begin{aligned} f_{\mathbf{s}_i}(\boldsymbol{\omega}, \tau) &= \gamma_i (\alpha_i^2 \beta_i^2 + \beta_i^2 |\boldsymbol{\omega}|^2 + \alpha_i^2 \tau_i^2 + |\boldsymbol{\omega}|^2 \tau^2)^{-\nu_i} \\ &= \gamma_i (\alpha_i^2 + |\boldsymbol{\omega}|^2)^{-\nu_i} (\beta_i^2 + \tau_i^2)^{-\nu_i}. \end{aligned}$$

Therefore the corresponding spatial-temporal covariance is separable, both spatial component and temporal component are Matérn type covariances.

Nonseparable and nonstationary models

When $\epsilon = 1$, $\gamma_i = \alpha_i = \beta_i = d = 1$ and $\nu = 3/2$, a contour plot of the corresponding separable spatial-temporal covariance is given here. There are sharp ridges.



Nonseparable and nonstationary models

When $\epsilon = 0$,

$$f_{\mathbf{s}_i}(\boldsymbol{\omega}, \tau) = \gamma_i (\alpha_i^2 \beta_i^2 + \beta_i^2 |\boldsymbol{\omega}|^2 + \alpha_i^2 |\tau|^2)^{-\nu_i}.$$

This is an extension of traditional Matérn spectral density. The parameter α_i^{-1} explains the rate of decay of the spatial correlation. For the temporal correlation, the rate of decay is explained by the parameter β_i^{-1} , γ_i is a scale parameter. The corresponding spatial-temporal covariance is a 3-d Matérn type covariance with an extra parameter, which can be considered a conversion factor between the units in the space and time domains.

Nonseparable and nonstationary models

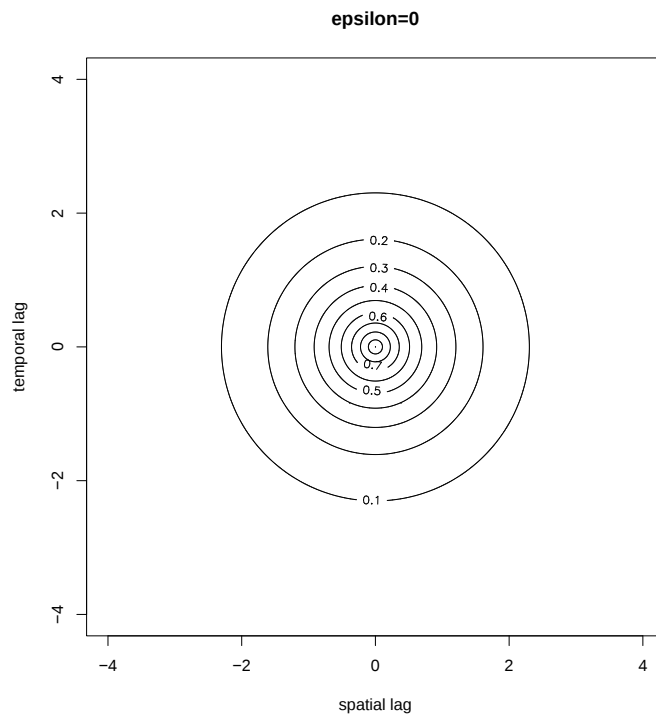
When $\epsilon = 0$,

$$C(\mathbf{x}, t) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\|(\mathbf{x}, \rho t)\|}{r} \right) \mathcal{K}_\nu \left(\frac{\|(\mathbf{x}, \rho t)\|}{r} \right),$$

- r is the range.
- σ^2 is the sill.
- $\nu > 0$ measures the smoothness of Z .
- ρ , which is new, is a scale factor to take into account the change of units between the spatial and temporal domains.
- This is a $d + 1$ Matérn type covariance, but it takes into account the change of units between space domain and temporal domain.

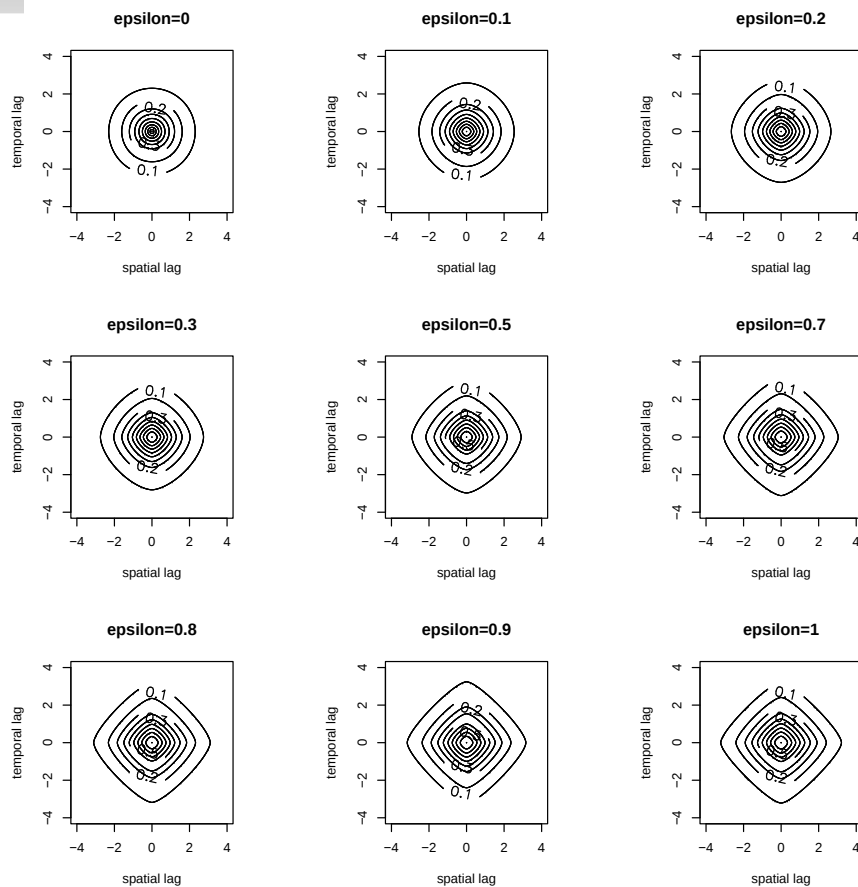
Nonseparable and nonstationary models

When $\epsilon = 0$, $\gamma = \alpha = \beta = d = 1$ and $\nu = 3/2$, a contour plot of corresponding separable spatial-temporal covariance is given here. It does not have ridges.



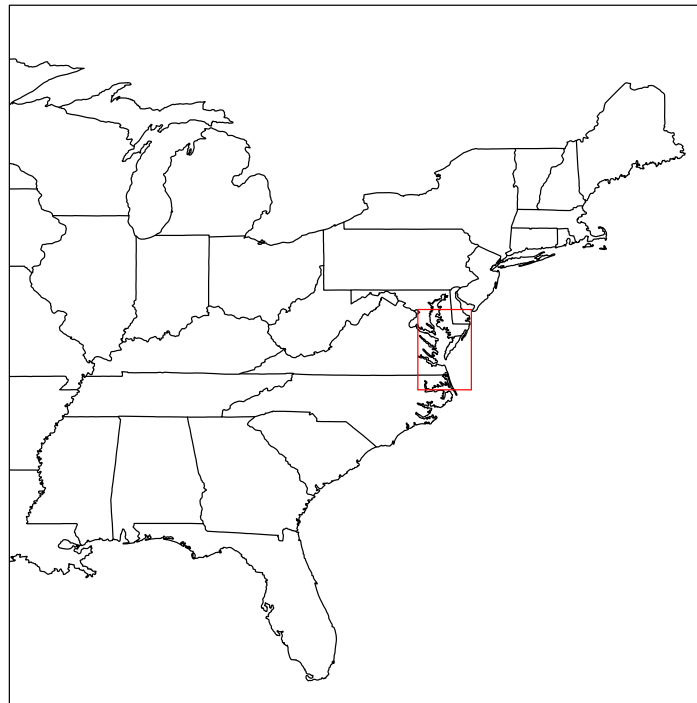
Nonseparable and nonstationary models

Space-time covariances for different values of ϵ ,



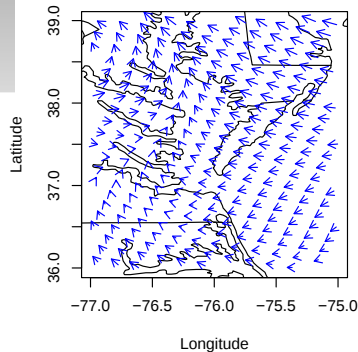
Spatiotemporal covariances for wind fields.

***Fuentes, Li and Davis (2005). The Chesapeake Bay (US).
Variable of interest: wind speed. July 21-24 2002 (there were
daily forced winds). Fuentes et al., (2004).***

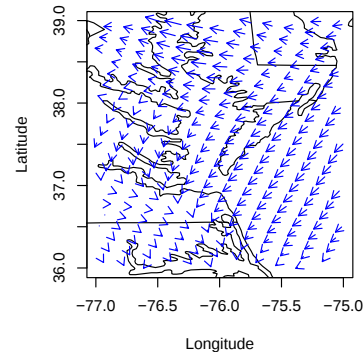


Spatiotemporal covariances for wind fields.

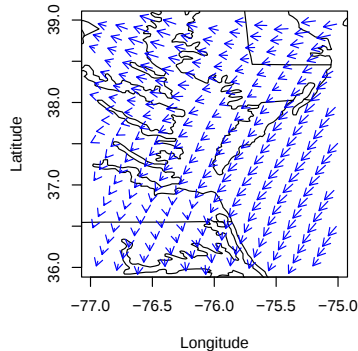
MM5 wind field at 3:00am,07-21-02



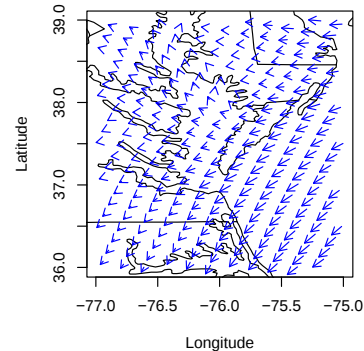
MM5 wind field at 6:00am,07-21-02



MM5 wind field at 9:00am,07-21-02

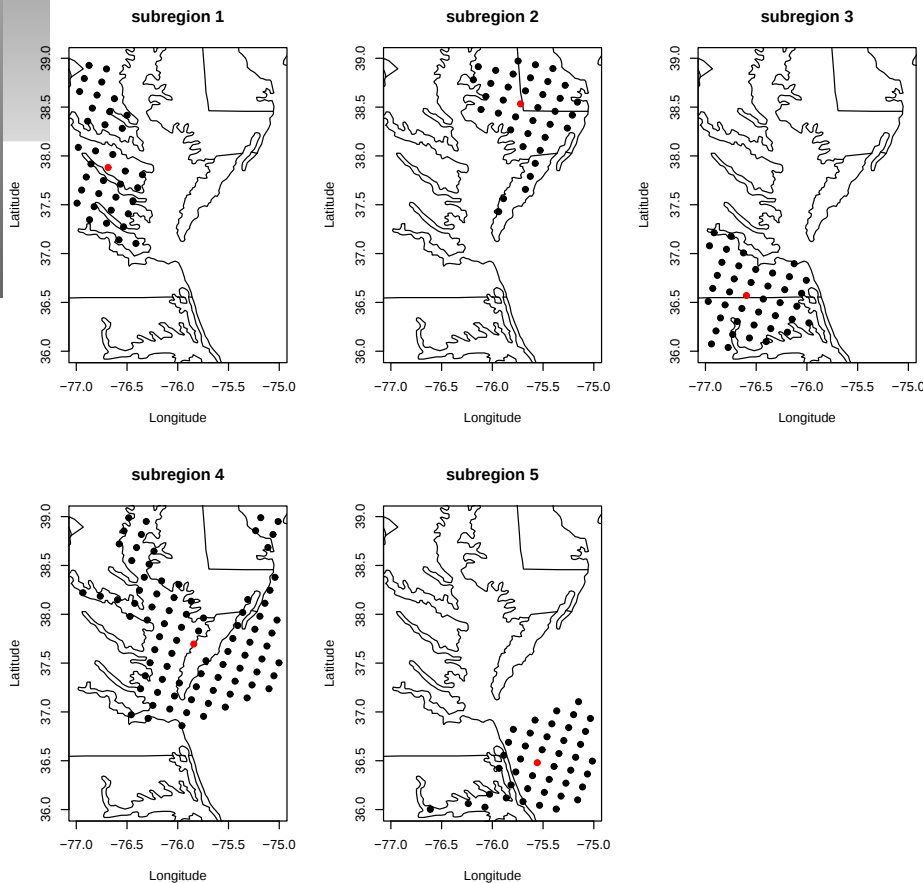


MM5 wind field at 12:00pm,07-21-02



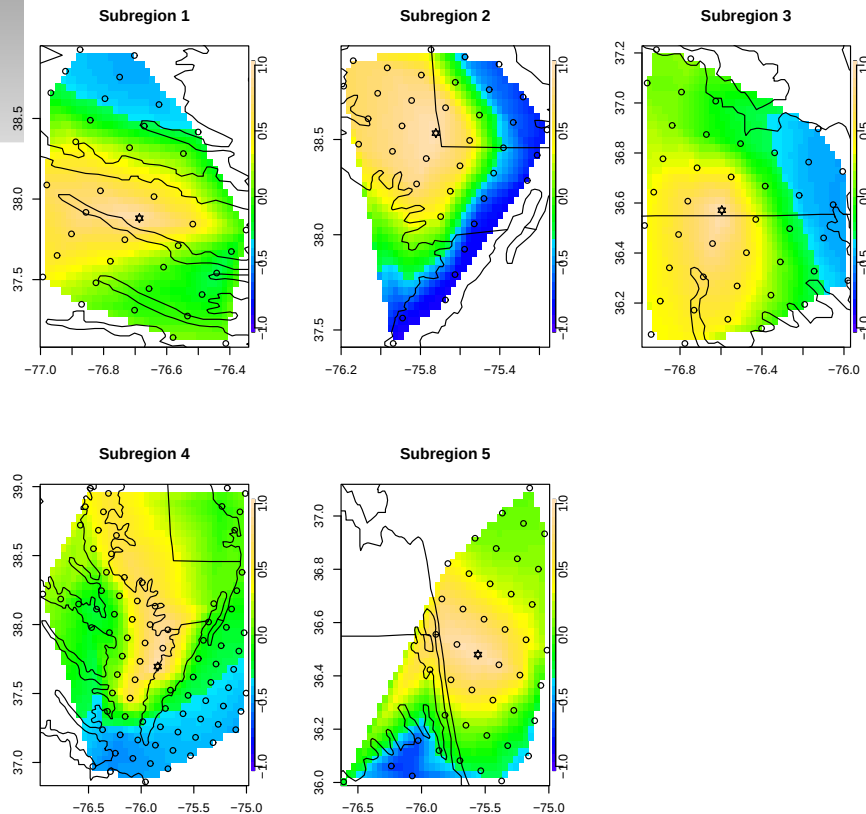
Grid for the output of MM5 in the Chesapeake Bay. We work with hourly data, 15km spatial resolution. We use MM5 36 hours forecast.

Spatiotemporal covariances for wind fields.



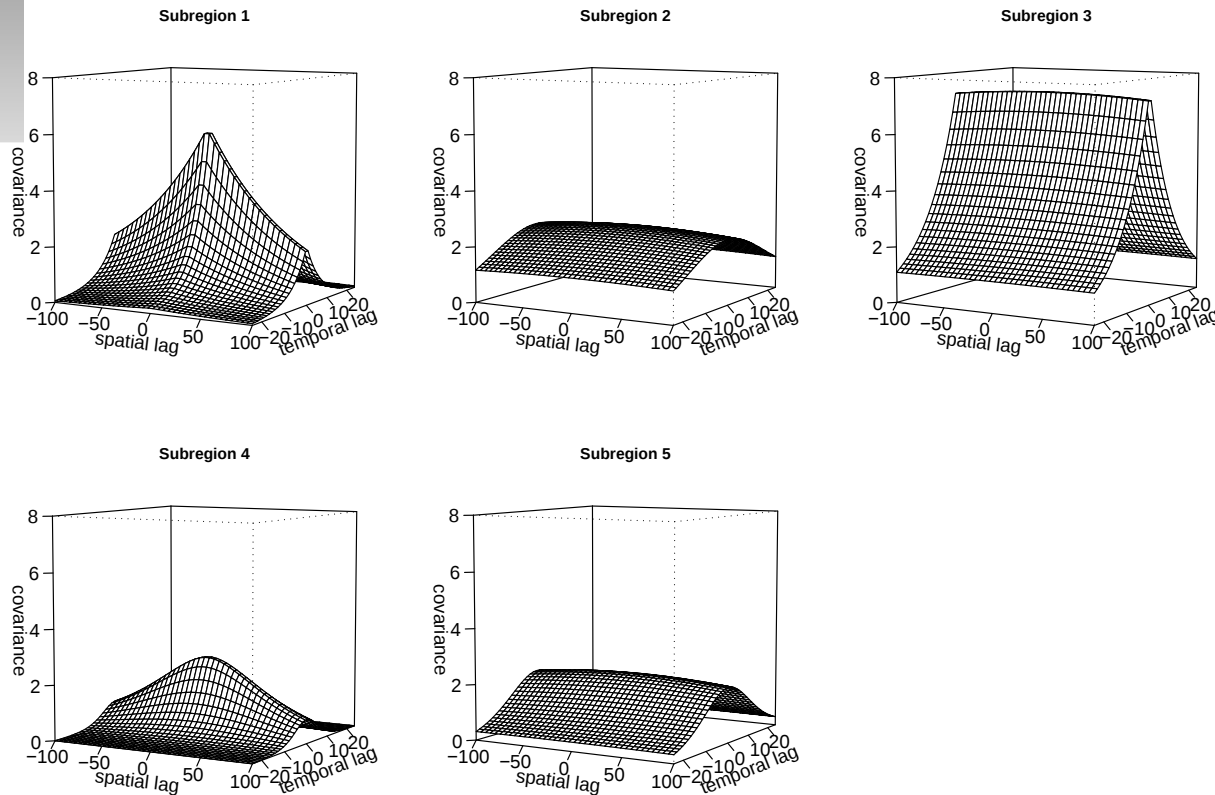
Subregions of stationarity (we used test for stationarity proposed by Fuentes (2002c)).

Spatiotemporal covariances for wind fields.



Correlation between each centroid and the other points within the subregion of stationarity at 12:00 pm on July 21, 2002.

Spatialtemporal covariances for wind fields.



Bayesian parametric estimates for the nonstationary and nonseparable covariance. *Units:* spatial distances in km, Time in hours, wind speed in meters/second.

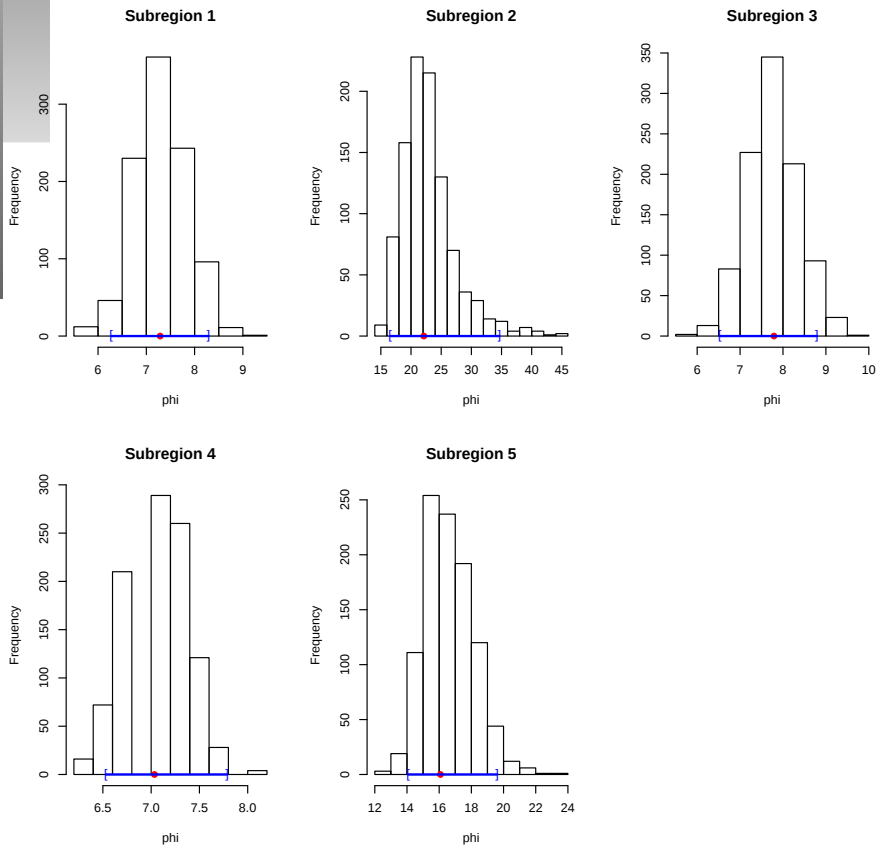
Spatiotemporal covariances for wind fields.

The posterior distributions for ϵ_i suggest the separability for each subregion except for subregion 4.

	$P(\epsilon_i = 0)$	$P(\epsilon_i = 1)$
Subregion 1	7.62e-48	1
Subregion 2	1.03e-91	1
Subregion 3	3.76e-94	1
Subregion 4	1	0
Subregion 5	2.56e-150	1

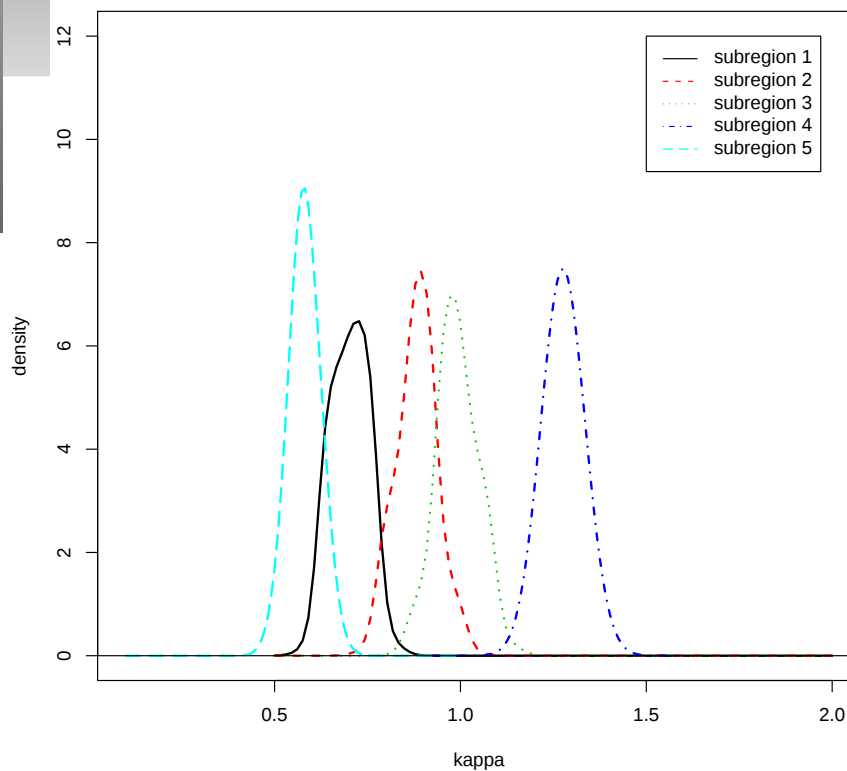
Table 1: The posterior distribution for ϵ_i .

Spatialtemporal covariances for wind fields.



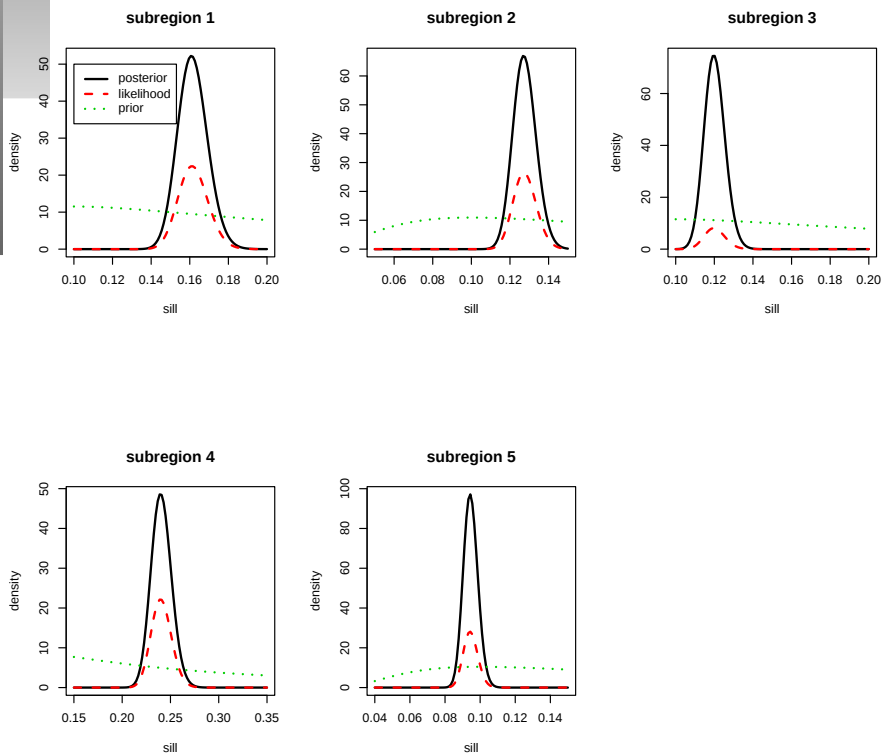
Posterior for the spatial range parameter.

Spatiotemporal covariances for wind fields.



Posterior for the smoothness parameter.

Spatialtemporal covariances for wind fields.



Posterior for the sill parameter.

Change of Support

The change-of-support problem occurs when the supports of predictand and data are not same. Here we are interested in making predictions about the random process at a point location $Z(\mathbf{x}_0)$ from data on block averages, $\tilde{Z}(B_1), \dots, \tilde{Z}(B_N)$.

We observe $\tilde{Z}$, the output of Models-3, averaged over regions, $B_1, \dots, B_N$, of dimensions $36\text{km} \times 36\text{km}$, and we want to predict Z (the true underlying process) at a location of interest $\mathbf{x}_0$.

Change of Support

The covariance for the block averages is defined as

$$\begin{aligned} \text{cov}(\tilde{Z}(B_{j_1}), \tilde{Z}(B_{j_2})) = \\ \int_{B_{j_1}} \int_{B_{j_2}} \text{cov}(\tilde{Z}(\mathbf{u}), \tilde{Z}(\mathbf{v})) d\mathbf{u} d\mathbf{v} = \\ b^2 \frac{\int_{B_{j_1}} \int_{B_{j_2}} C(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta}) d\mathbf{u} d\mathbf{v}}{|B_{j_1}| |B_{j_2}|} + \mathbf{1}_{\{j_1=j_2\}} \sigma_\delta^2 |B_{j_1}| \end{aligned}$$

where $C(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta})$ is the covariance for the true underlying process Z , and $\boldsymbol{\theta}$ is the covariance parameter. We model C as a **nonstationary** spatial function.

Change of Support

We define the process Z in terms of a **pointwise covariance** $C(\mathbf{u}, \mathbf{v})$, but we then use the previous expression to derive the covariances of the block averages $\tilde{Z}(B_i)$, $i = 1, \dots, N$, in terms of the pointwise covariance $C(\mathbf{u}, \mathbf{v})$.

This is then used to define a **likelihood** function for the parameters of the covariance function for the process Z in terms of the observed block averages $\tilde{Z}(B_1), \tilde{Z}(B_2), \dots, \tilde{Z}(B_N)$.

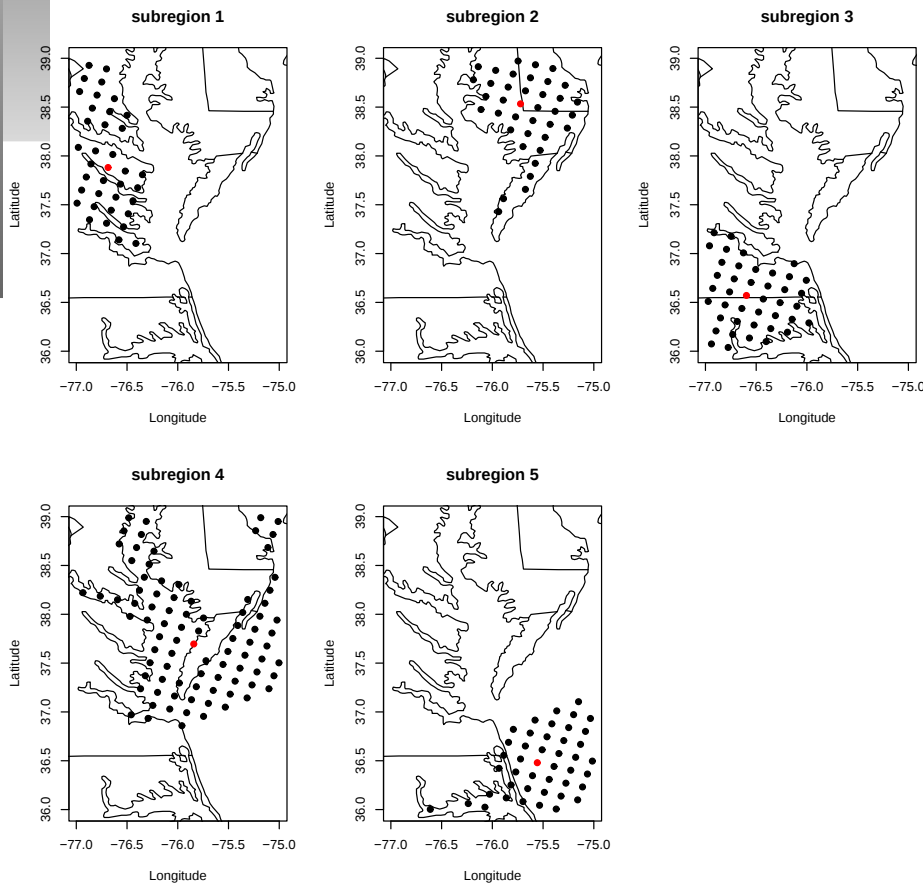
Application: Wind field estimation.

We use the Hierarchical Bayesian melding approach to combine MM5 output ($\tilde{Z}$) and monitoring data ($\hat{Z}$) to improve space-time trend and covariance estimation for wind fields over the Chesapeake bay. We only used geographic information (no covariates).

The underlying truth Z is a stochastic process with a space-time μ large scale structure, and a nonseparable and nonstationary covariance for the error term η .

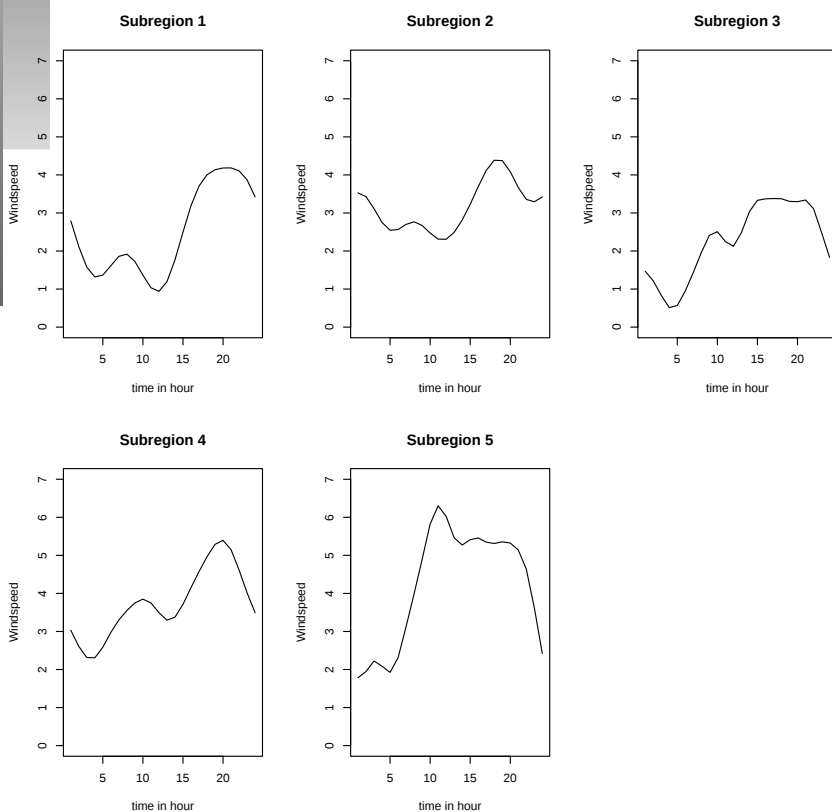
μ is modeled using sine and cosine functions with spatially varying coefficients (different temporal trend for different subregions in our domain).

Application: Wind field estimation.



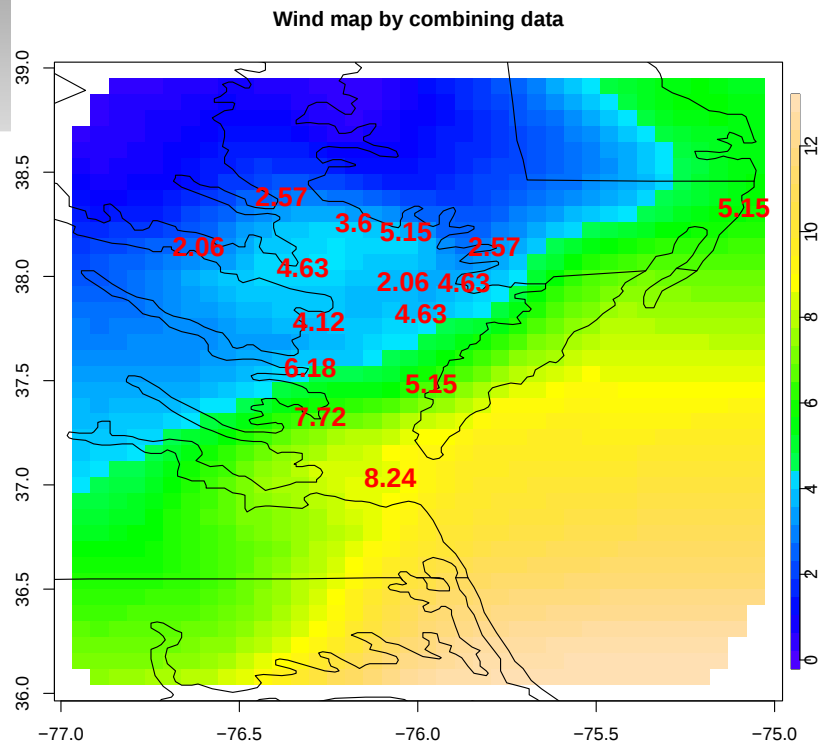
Subregions of stationarity (determined using a test for stationarity).

Application: Wind field estimation.



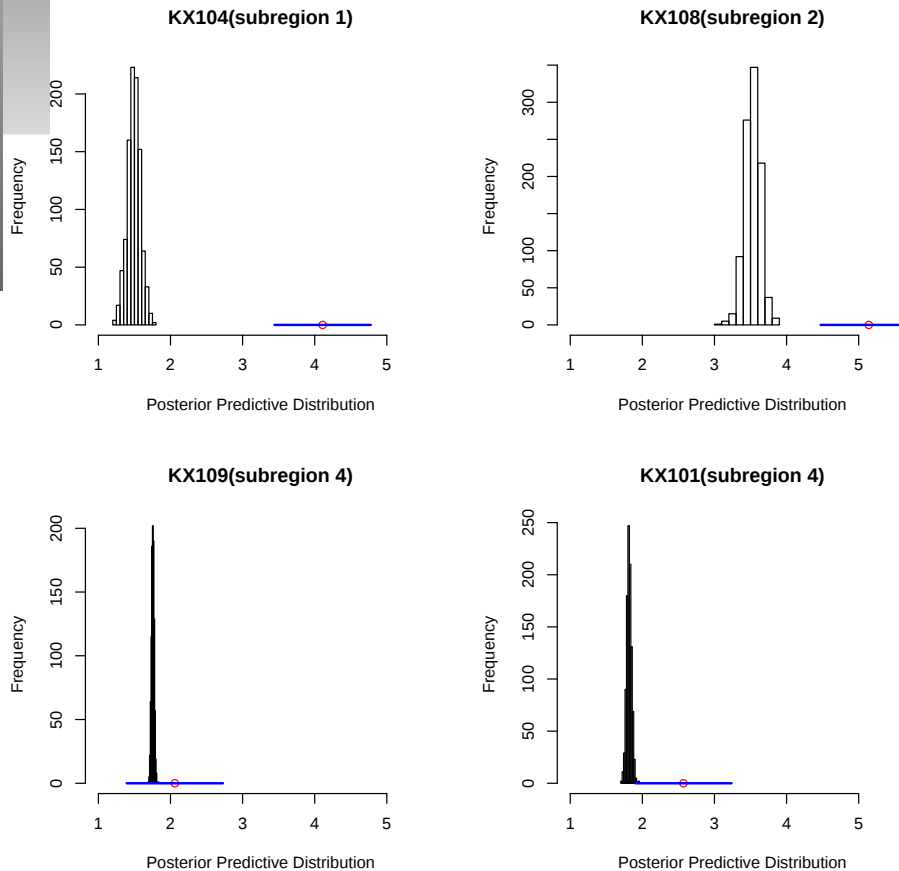
Graph of μ for the wind speed. Estimated temporal trends for each subregion combining model output and monitoring data. The solid line shows the trend for each of the 5 subregions of stationarity for July 21 2002.

Application: Wind field estimation.



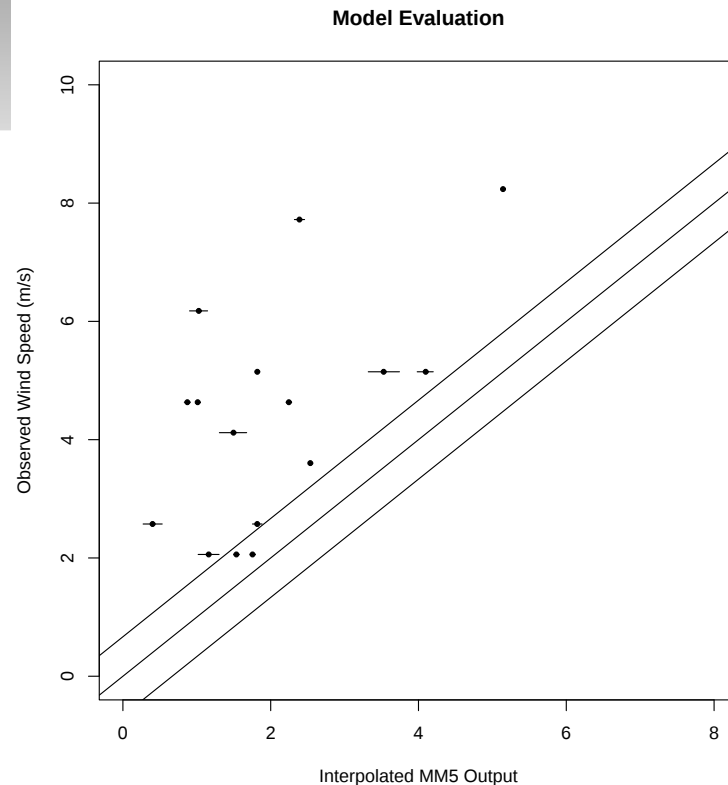
Improved wind fields maps, by combining MM5 and observations at 12:00 pm on July 21, 2002. .

Application: Wind field estimation.



ppd of MM5 at the locations where we have data, at 12:00 pm on July 21, 2002. The red dot is the observed value (with a 95% CI).

Application: Wind field estimation.



Median of the ppd of MM5 at the locations where we have data (horizontal axis) versus the observed data (vertical axis), 12:00 pm on July 21, 2002. Overall, MM5 seems to underestimate the wind speed values.

Diagnostics: Wind field estimation.

- **Define $MSE = \frac{1}{n} \sum_{i=1}^n (\hat{r}_{-i} - r_{oi})^2$, r_{oi} is the observed wind speed at location i , $\hat{r}_{-i}$ is the predicted value at location i (without using r_{oi}) and n is the number of observations.**

3D-Var:

$$Z = \tilde{Z} + W[\hat{Z} - H(\tilde{Z})],$$

where

- $W = BH^T(R + HBH^T)^{-1}$,
- B is error covariance matrix for MM5,
- R is error cov. matrix for observations,
- and H is an operator to interpolate MM5 to the observational sites.

Diagnostics: Wind field estimation.

	MM5	New	3D-Var
noon	10.32	2.448	9.176
6pm	8.941	4.726	5.158

Table 2: The comparison of MSEs (m/s^2).

- Improved wind map can be obtained by combining observed wind data with MM5 model output.
- However, these results are based on a very limit time period.

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