An Overview of Nonstationary Spatial Modeling

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Nonstationary Spatial Modeling

A GENERAL MODELING FRAMEWORK

- Let $Z(\cdot)$ be a realization of a spatial stochastic process defined for all $\boldsymbol{s} \in \mathcal{D} \subset \mathbb{R}^d$, where d is typically equal to 2 or 3
- We observe the value of $Z(\cdot)$ at a finite set of locations $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n \in \mathcal{D}$ and wish to learn about the underlying process
- For all $\boldsymbol{s} \in \mathcal{D}$, let

$$Z(\boldsymbol{s}) = \mu(\boldsymbol{s}) + Y(\boldsymbol{s}) + \epsilon(\boldsymbol{s})$$

  where

  - $\mu(\cdot)$ is a deterministic mean function
  - $Y(\cdot)$ is a mean-zero latent spatial (Gaussian) process
  - $\epsilon(\cdot)$ is a spatially independent error process, which is assumed to be independent of $Y(\cdot)$

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Definition A process is said to be second-order stationary if

$$\mathrm{E}[Y(\boldsymbol{s})] = \mathrm{E}[Y(\boldsymbol{s}+\boldsymbol{h})] = \text{ constant}$$

and

$$\mathrm{cov}[Y(\boldsymbol{s}), Y(\boldsymbol{s}+\boldsymbol{h})] = \mathrm{cov}[Y(\boldsymbol{0}), Y(\boldsymbol{h})] = C(\boldsymbol{h})$$

where the function $C(\boldsymbol{h})$, $\boldsymbol{h} \in \mathbb{R}^d$ is called the covariance function

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- Is second-order stationarity a "reasonable" assumption?

  $\rightarrow$ $\mathrm{E}[Y(\boldsymbol{s})] = \mathrm{E}[Y(\boldsymbol{s}+\boldsymbol{h})] =$ constant?

  $\rightarrow$ $\mathrm{cov}[Y(\boldsymbol{s}), Y(\boldsymbol{s}+\boldsymbol{h})] = \mathrm{cov}[Y(\boldsymbol{0}), Y(\boldsymbol{h})] = C(\boldsymbol{h})$?

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- How might one check whether the assumption is reasonable?

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- Here, $Y(\cdot)$ is a nonstationary spatial process with covariance function $C(\boldsymbol{s}_1, \boldsymbol{s}_2) = \text{cov}(Y(\boldsymbol{s}_1), Y(\boldsymbol{s}_2))$
- We focus on modeling $C(\boldsymbol{s}_1, \boldsymbol{s}_2)$:
  1. has to be a valid covariance function
  2. has to be estimable (perhaps from only a single realization of the process)
- Following Sampson (2010)'s categorization, the following are a few approaches in the literature:
  1. Smoothing and weighted-average methods
  2. Basis function methods
  3. Process convolutions / spatially-varying parameters
  4. Deformations

  ... and possibly others?

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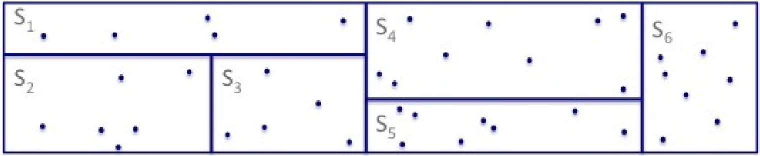
1. SMOOTHING / WEIGHTED-AVERAGE METHODS

Idea: Construct a nonstationary spatial process by smoothing several locally stationary processes

An example: (Fuentes, 2001):

- Divide the spatial region $\mathcal{D}$ into k disjoint subregions S_i, for $i = 1, \ldots, k$, such that $\mathcal{D} = \cup_{i=1}^{k} S_i$
- Let $Y_1(\cdot), Y_2(\cdot), \ldots, Y_k(\cdot)$ be stationary spatial processes associated with each of the subregions, with covariance functions estimated using the observations in each subregion



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- Construct a global nonstationary process as a weighted average of the locally stationary processes:

$$Y(\boldsymbol{s}) = \sum_{i=1}^{k} w_i(\boldsymbol{s}) Y_i(\boldsymbol{s}),$$

  where $w_i(\boldsymbol{s})$ is weight function based on the distance between $\boldsymbol{s}$ and the 'center' of region S_i

- The number of subregions is chosen using BIC

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Some other approaches:

- Fuentes and Smith (2002) propose a continuous extension of the original model where

$$Y(\boldsymbol{s}) = \int_{\mathcal{D}} w(\boldsymbol{s} - \boldsymbol{u}) Y_{\theta(u)}(\boldsymbol{s}) d\boldsymbol{u}$$

- Nott and Dunsmuir (2002) propose letting

$$C(Y(\boldsymbol{s}_1), Y(\boldsymbol{s}_2)) = \Sigma_0 + \sum_{i=1}^{k} \underbrace{w_i(\boldsymbol{s}_1) w_i(\boldsymbol{s}_2) C_{\theta_i}(\boldsymbol{s}_1 - \boldsymbol{s}_2)}_{\text{local } \textit{residual} \text{ covariance structure}}$$

- Guillot et al. (2001) propose a nonparametric kernel estimator of a nonstationary covariance matrix

- Kim, Mallick, and Holmes (2005)'s approach automatically partitions the spatial domain into disjoint regions and then fits a piecewise Gaussian process model

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2. BASIS FUNCTION MODELS

Idea: decompose the spatial covariance function in terms of basis functions

An example: EOFs

- The Karhunen-Loéve (K-L) expansion of a covariance function is

$$C_Y(\boldsymbol{s}_1, \boldsymbol{s}_2) = \sum_{k=1}^{\infty} \lambda_k \phi_k(\boldsymbol{s}_1)\phi_k(\boldsymbol{s}_2)$$

  where $\{\phi_k(\cdot) : k = 1, \ldots, \infty\}$ and $\{\lambda_k : k = 1, \ldots, \infty\}$ are the eigenfunctions and eigenvalues, respectively, of the Fredholm integral equation:

$$\int_{\mathcal{D}} C_Y(\boldsymbol{s}_1, \boldsymbol{s}_2)\phi_k(\boldsymbol{s})d\boldsymbol{s} = \lambda_k \phi_k(\boldsymbol{s}_2)$$

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- Using this expansion, we can write the process as

$$Y(\boldsymbol{s}) = \sum_{k=1}^{\infty} a_k \phi_k(\boldsymbol{s}).$$

- It can be shown that the truncated decomposition

$$Y_p(\boldsymbol{s}) = \sum_{k=1}^{p} a_k \phi_k(\boldsymbol{s})$$

  is optimal in the sense that it minimizes the variance of the truncation error among all sets of basis function representations of $Y(\cdot)$ of order p.

- The $\phi_k(\boldsymbol{s})$s can be obtained numerically by solving the Fredholm integral equation (can be difficult).

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- An alternative solution when repeated observations of the spatial process (e.g., over time) are available: perform a principal components analysis of the empirical covariance matrix

  That is, if $\boldsymbol{S}$ is the empirical covariance matrix, we can solve the eigensystem

  $$\boldsymbol{S}\boldsymbol{\Phi} = \boldsymbol{\Phi}\boldsymbol{\Lambda},$$

  where

  - $\boldsymbol{\Phi}$ is the matrix of eigenvectors $\rightarrow$ called the "empirical orthogonal functions" or EOFs

  - $\boldsymbol{\Lambda}$ is the diagonal matrix with corresponding eigenvalues on the diagonal

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- We can use $\mathbf{\Phi}\boldsymbol{\alpha}$ in place of $\boldsymbol{Y} = (Y(\boldsymbol{s}_1), \ldots, Y(\boldsymbol{s}_n))'$, where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)'$ are a collection of unknown parameters

  $\rightarrow$ a truncated version of this representation is used for dimension reduction

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Advantages of using EOFs:

1. naturally nonstationary

Disadvantages of using EOFs:

1. prediction
2. measurement error

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Some other examples:

- Holland et al. (1998) represents a nonstationary spatial covariance function as the sum of a stationary model and a finite sum of EOFs
- Nychka (2002) uses multiresolution wavelets instead of EOFs for computational reasons. More recent work by Matsuo, Nychka, and Paul (2008) has extended the approach to handle irregularly spaced data
- Pintore and Holmes (2004) and Stephenson et al. (2005) induce nonstationarity by evolving the stationary power spectrum with a latent spatial power process
- Katzfuss (2014) propose a model with a low-rank representation of a nonstationary Matérn (with covariance tapering) model for computational considerations

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3. PROCESS CONVOLUTION MODELS / SPATIALLY-VARYING PARAMETERS

Idea: use a constructive specification of a (Gaussian) process to introduce nonstationarity

An example: (Higdon, 1998)

- Let $k(\cdot) : \mathbb{R}^d \to \mathbb{R}$ be a function satisfying

$$\int_{\mathbb{R}^d} k(\boldsymbol{u}) d\boldsymbol{u} < \infty \quad \text{and} \quad \int_{\mathbb{R}^d} k^2(\boldsymbol{u}) d\boldsymbol{u} < \infty$$

  and $W(\cdot)$ denote d-dimensional Brownian motion.

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- It can be shown that the process

$$Y(\boldsymbol{s}) = \int_{\mathbb{R}^d} k_{\boldsymbol{s}}(\boldsymbol{u}) W(d\boldsymbol{u})$$

  is Gaussian with $\mathrm{E}[Y(\boldsymbol{s})] = 0$ and

$$C_Y(\boldsymbol{s}_1, \boldsymbol{s}_2) = \mathrm{cov}[Y(\boldsymbol{s}_1), Y(\boldsymbol{s}_2)] = \int_{\mathbb{R}^d} k_{\boldsymbol{s}_1}(\boldsymbol{u}) k_{\boldsymbol{s}_2}(\boldsymbol{u}) d\boldsymbol{u}$$

  for $\boldsymbol{s} \in \mathcal{D} \subset \mathbb{R}^d$

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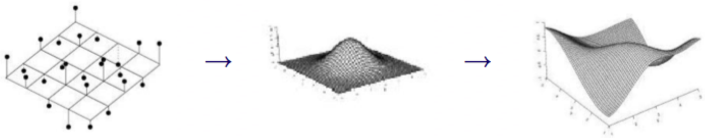
- Higdon (1998) proposes a discrete approximation to a nonstationary Gaussian process:

$$Y(\boldsymbol{s}) = \sum_{i=1}^{k} k_{\boldsymbol{s}}(\boldsymbol{u}_i)\, x_i$$

where the x_i's are i.i.d. $\mathrm{N}(0, \lambda^2)$ random variables associated with each knot location $\boldsymbol{u}_i$.



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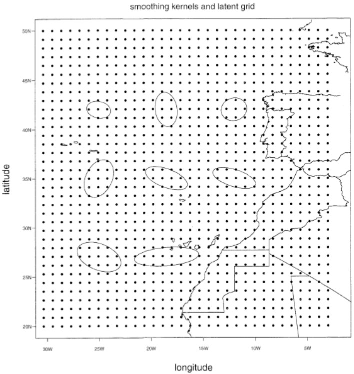
- Higdon (1998) proposes using this model for North Atlantic ocean temperatures. In this model, the kernels were weighted averages of fixed 'basis kernels'

$$Y(\boldsymbol{s}) = \sum_{i=1}^{k} k_{\boldsymbol{s}}(\boldsymbol{u}_i)\, x_i$$

where

$$k_{\boldsymbol{s}}(u_i) = \sum_{j=1}^{8} w_j(\boldsymbol{s}) k_{\boldsymbol{s}_j^*}(\boldsymbol{u}_i)$$

$$w_j(\mathbf{s}) \propto \exp\left(-\frac{1}{2}||\boldsymbol{s} - \boldsymbol{s}_{\mathbf{j}}^*||^2\right)$$



(Higdon, 1998)

$$k_{\boldsymbol{s}_j^*}(\boldsymbol{u}_i) = \frac{1}{\sqrt{2\pi}} |\boldsymbol{\Sigma}_{\boldsymbol{s}_j^*}|^{-1} \exp\left(-\frac{1}{2}(\boldsymbol{s}_j^* - \boldsymbol{u}_i)' \boldsymbol{\Sigma}_{\boldsymbol{s}_j^*}^{-1} (\boldsymbol{s}_j^* - \boldsymbol{u}_i)\right)$$

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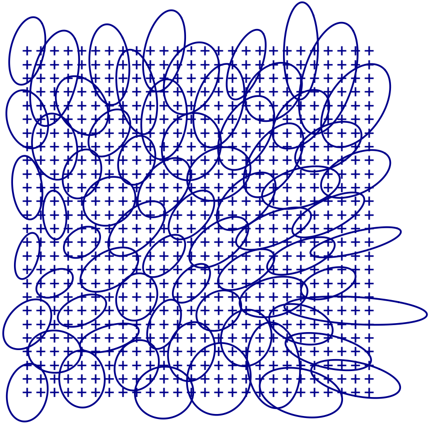
Some other examples:

- Kernel parameters can vary smoothly in space (Higdon, Swall, and Kern, 1999; Paciorek and Schervish, 2006):



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- Paciorek and Schervish (2006) use this idea to develop a general class of nonstationary covariance functions (including the Matérn model):

$$C(\boldsymbol{s}_1, \boldsymbol{s}_2) = \sigma^2 |\boldsymbol{\Sigma}_1|^{1/4} |\boldsymbol{\Sigma}_2|^{1/4} \left| \frac{\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2}{2} \right|^{-1/2} g(-\sqrt{Q_{12}})$$

  where

$$Q_{12} = (\boldsymbol{s}_1 - \boldsymbol{s}_2)' \left(\frac{\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2}{2} \right)^{-1} (\boldsymbol{s}_1 - \boldsymbol{s}_2)$$

  and $g(\cdot)$ is a valid isotropic correlation function

  This model allows locally-varying geometric anisotropies $\rightarrow$ more on this model in the practicum

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- Stein (2005) and Anderes and Stein (2011) extend the Paciorek and Schervish (2006) model to allow spatially-varying variance and smoothness parameters
- Kleiber and Nychka (2012) further extend this model to the multivariate setting
- Calder (2007, 2008) proposes space-time versions of the Hidgon model
- Heaton (2014) extends process convolution models to spherical spatial domains

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3. DEFORMATIONS

Idea: (Sampson and Guttorp, 1992): Map the geographic locations of observations to a deformed space where stationarity holds

A Bayesian example: (Schmidt and O'Hagan, 2003)

- Consider the $n \times n$ sample covariance matrix, $\boldsymbol{S}$, of a spatial process observed at n locations independently at T time points. The goal is to learn the true covariance matrix of the Gaussian process, $\boldsymbol{\Sigma}$, from $\boldsymbol{S}$.

- Likelihood function:

$$f(\boldsymbol{S}|\boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-(T-1)/2} \exp\left(-\frac{T}{2} tr(\boldsymbol{S}\boldsymbol{\Sigma}^{-1})\right)$$

- The diagonal elements of $\boldsymbol{\Sigma}$ are given conditionally independent inverse gamma priors.

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- The off diagonal elements of $\boldsymbol{\Sigma}$ are modeled as follows:

$$C_d(s_i, s_j) = g(||\boldsymbol{d}(\boldsymbol{x}_i) - \boldsymbol{d}(\boldsymbol{x}_j)||)$$

  where $g(\cdot)$ is a monotone function of the form

$$g(h) = \sum_{i=1}^{k} a_k \exp(-b_k h^2)$$

  with the a_k's and b_k's unknown.

- The $\boldsymbol{d}(\cdot)$ process:

$$\boldsymbol{d}(\cdot) \sim \mathrm{GP}(\boldsymbol{\mu}(\cdot), \boldsymbol{\sigma}_d^2 R_d(\cdot,\cdot))$$

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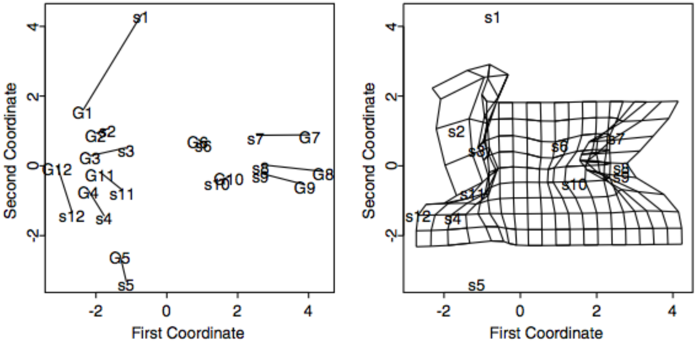
- Schmidt and O'Hagan claim that Gaussian process prior on the deformation process tends to eliminate the non-injective mappings noted by Sampson and Guttorp (1992).



(Schmidt and O'Hagan, 2003)

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SUMMARY

- lots of models $\rightarrow$ some have been well studied, some haven't
- very little work on model comparison
- with the exception of the basis function models, computation is a BIG challenge
- no general software
- recent work has focused on understanding the reasons for nonstationarity (e.g., covariates)
- nonstationary versus non-Gaussian models

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