Stochastic Local Interaction Models for Processing Spatiotemporal Datasets

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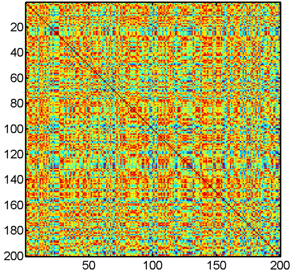
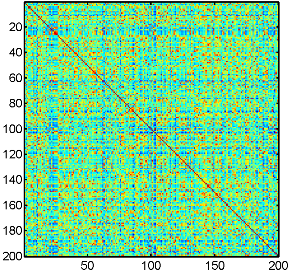
Motivation: Geostatistics and Gaussian Process Regression face challenges for $N \gg 1$



Dense Covariance matrix



Dense Precision matrix

Problem: Inversion of large (for $N \gg 1$), dense covariance matrices
Problem: Covariance functions are mathematical constructions typically lacking physical motivation

Motivation: Geostatistics and Gaussian Process Regression face challenges for $N \gg 1$

- Best Linear Unbiased Estimator (BLUE) (a.k.a. Ordinary Kriging)

$$\hat{X}(\mathbf{s}) = \sum_{j=1}^{m} \lambda_j X(\mathbf{s}_j), \quad \mathbf{s}_j \in B(\mathbf{s}; r_c), \; B(\cdot;\cdot) : \text{search neighborhood}$$

- *Best*: minimum mean square estimation error

$$\{\lambda_1, \lambda_2, \ldots, \lambda_m\} = \arg \min_{\lambda_1,\lambda_2,\ldots,\lambda_m} \left(\mathbb{E}\left\{ \hat{X}(\mathbf{s}) - X(\mathbf{s}) \right\}^2 \Big| \; \lambda_1 + \lambda_2 + \ldots \lambda_m = 1 \right)$$

- Spatial weights follow from the linear system: $\mathbf{C}_{N,N}\, \boldsymbol{\Lambda} = \mathbf{C}_{N,0}$

$$\begin{bmatrix} c(\mathbf{s}_1-\mathbf{s}_1) & c(\mathbf{s}_1-\mathbf{s}_2) & \ldots & c(\mathbf{s}_1-\mathbf{s}_m) & 1 \\ c(\mathbf{s}_2-\mathbf{s}_1) & c(\mathbf{s}_2-\mathbf{s}_2) & \ldots & c(\mathbf{s}_2-\mathbf{s}_m) & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c(\mathbf{s}_m-\mathbf{s}_1) & c(\mathbf{s}_m-\mathbf{s}_2) & \vdots & c(\mathbf{s}_m-\mathbf{s}_m) & 1 \\ 1 & 1 & \ldots & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_m \\ \mu \end{bmatrix} = \begin{bmatrix} c(\mathbf{s}_1-\mathbf{s}) \\ c(\mathbf{s}_2-\mathbf{s}) \\ \vdots \\ c(\mathbf{s}_m-\mathbf{s}) \\ 1 \end{bmatrix}$$

Introduction

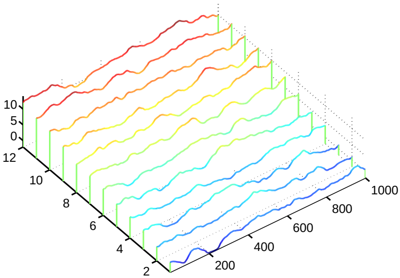
- Ideas inspired from Statistical Physics can help to model efficiently spatiotemporal data
- There is a long history of interplay between statistical physics and statistical data analysis (*Ising model, Markov Chain Monte Carlo, Metropolis updating, variational Gaussian approximations in machine learning, etc.*)
- The main themes for this presentation are:

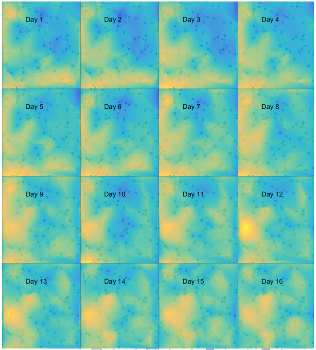
  (i) Construction of *stochastic local interaction* computationally efficient models for space-time data analysis

  (ii) Application to natural resources and environmental data

Representations of Space-Time Random Fields

- In simple terms, an STRF $X(\mathbf{s}, t; \omega)$ is *an ensemble* (collection) of functions $x(\mathbf{s}, t)$ where $\mathbf{s} \in \mathbb{R}^d$ and $t \in T \subset [0, \infty)$.
- The index ω distinguishes different states (functions). In practice it is often suppressed.





Representations of Space-Time Random Fields

- The classical case: Joint probability density function of Gaussian data in terms of the covariance matrix **C**

$$f_{\mathrm{X}} \propto \exp\left(-\frac{1}{2}\sum_{i,j=1}^{N} x_i\, C^{-1}_{x;\,i,j}\, x_j\right) \; ; \quad C_{x;\,i,j} : \text{ Covariance matrix}$$

- The Boltzmann-Gibbs representation: Joint probability density function based on an "energy function" with controlled space-time structure

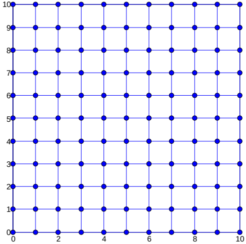
$$f[x(\mathbf{s})] = Z(\boldsymbol{\theta})^{-1}\, \mathrm{e}^{-\mathcal{H}[x(\mathbf{s};\boldsymbol{\theta})]}, \; \mathcal{H}[x(\mathbf{s})] : \text{ energy functional,}$$

- $Z(\boldsymbol{\theta})$: partition function is a normalizing factor

Local Interactions on Rectangular Grids

Grid structure: SSRFs ⇒ Gauss-Markov random fields

$$\mathcal{H}[x(\mathbf{s})] = \lambda \sum_{n=1}^{N} \left\{ [x(\mathbf{s}_n) - m_x]^2 + c_1 \sum_{i=1}^{d} \left[\frac{x(\mathbf{s}_n + a_i\,\hat{\mathbf{e}}_i) - x(\mathbf{s}_n)}{a_i} \right]^2 + c_2 \sum_{i=1}^{d} \left[\frac{x(\mathbf{s}_n + a_i\,\hat{\mathbf{e}}_i) - 2x(\mathbf{s}_n) + x(\mathbf{s}_n - a_i\,\hat{\mathbf{e}}_i)}{a_i^2} \right]^2 \right\}$$



$\hat{\mathbf{e}}_i,\ i = 1, \ldots, d$: unit vectors in lattice directions

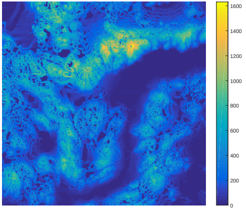
a_i : lattice steps

$$\mathcal{H}_{fgc}[X(\mathbf{s})] = \lambda S_0 + c_1\, \lambda\, S_G + c_2\, \lambda\, S_c$$

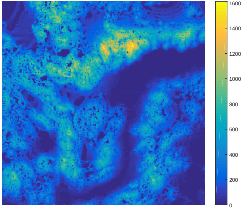
Rue and Held, *Gaussian Markov Random Fields: Theory and Applications*, Chapman and Hall/CRC, 2005

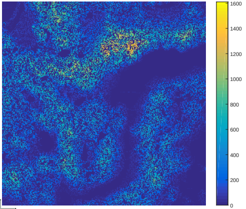
Reconstruction of Walker Lake Data (260 × 300 grid)

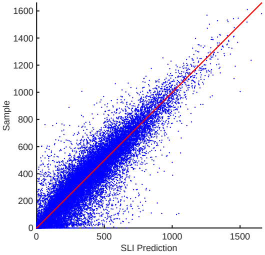
Anisotropic model based on 39 000 sampling points (50%)

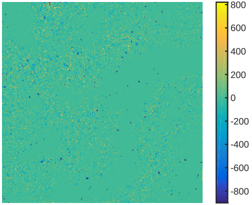


Left top: Full data set
Left bottom: Sample
Right top: SLI-based map
Right bottom: SLI spatial error



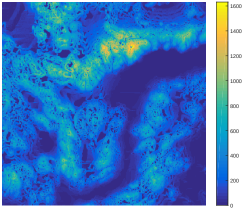


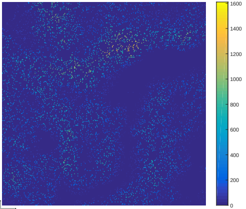




Reconstruction of Walker Lake Data (260 × 300 grid)

Anisotropic SLI model – 7 800 sampling points (10%)





Left top: Full data set
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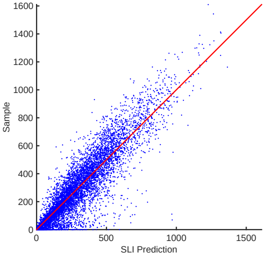
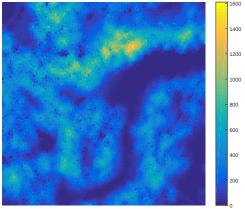
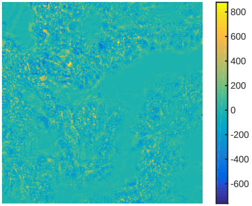






SLI Model for space-time data

- The vector $\mathbf{x}_{\mathbb{S}} \equiv (x_1, x_2, \ldots, x_N)^\top$ comprises the *observations* at the space-time point set $\mathbb{S}_N = \{(\mathbf{s}_1, t_1), (\mathbf{s}_2, t_2), \ldots (\mathbf{s}_N, t_N)\}$
- Energy function for *stochastic local interaction (SLI) model*

$$\mathcal{H}(\mathbf{x}_{\mathbb{S}}; \boldsymbol{\theta}) = \frac{1}{2\,\lambda} \left[\frac{{\mathbf{x}'_{\mathbb{S}}}^\top \mathbf{x}'_{\mathbb{S}}}{N} + c_1\, \mathcal{S}_1(\mathbf{x}'_{\mathbb{S}}; \mathbf{h}_s, \mathbf{h}_t) \right], \quad \mathbf{x}'_{\mathbb{S}} = \mathbf{x}_{\mathbb{S}} - \mathbf{m}_{\mathrm{x}}$$

- Local interactions are implemented by means of simple expressions that involve kernel-weighted averages [Hristopulos, 2015, Hristopulos & Agou, 2019]
- A crucial idea is that the kernel bandwidth is automatically adjusted to account for the local sampling density

SLI Model for space-time data

$$\mathcal{H}(\mathbf{x}_\mathrm{S};\boldsymbol{\theta}) = \frac{1}{2\,\lambda}\left[\frac{{\mathbf{x}'_\mathrm{S}}^\top \mathbf{x}'_\mathrm{S}}{N} + c_1\,\mathcal{S}_1(\mathbf{x}'_\mathrm{S};\mathbf{h}_s,\mathbf{h}_t)\right], \quad \mathbf{x}'_\mathrm{S} = \mathbf{x}_\mathrm{S} - \mathbf{m}_\mathrm{x}$$

SLI model parameters

- λ: Overall scale parameter
- c_1: Rigidity coefficient
- μ_s, K_s: Spatial kernel bandwidth: $h_{s,n} = \mu_s\, D_{n,[K_s]}(\mathbb{S}_N)$
- $D_{n,[K_s]}(\mathbb{S}_N)$: distance between $\mathbf{s}_n$ and K_s-nearest neighbor in $\mathbb{S}_N$
- μ_t, K_t: Temporal kernel bandwidth: $h_{t,n} = \mu_t\,(K_t - 1)\delta t$
- $\{\beta_k\}_{k=1}^{K}$: Coefficients of trend model $m_\mathrm{x}(\mathbf{s},t) = \sum_{k=1}^{K}\beta_k f_k(\mathbf{s},t)$

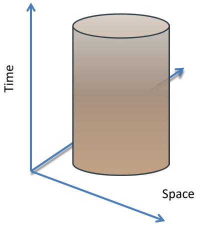
Different approaches for kernel weight selection

Separable space-time structure

$$w_{n,k} = K\left(\frac{\|\mathbf{r}_{n,k}\|}{h_{s,n}}\right) K\left(\frac{|\tau_{n,k}|}{h_{t,n}}\right)$$

This does not imply *separable covariance*

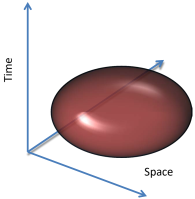
Currently we use this approach



Composite space-time metric

$$w_{n,k} = K\left(\frac{\sqrt{\mathbf{r}^2_{n,k} + \tau^2_{n,k}/\alpha^2}}{h_{s,n}}\right)$$

Relation of S-T bandwidths: $h_{t,n} = \alpha h_{s,n}$



SLI precision matrix formulation

Quadratic Form of SLI Energy: Sparse by Construction

$$\mathcal{H}(\mathbf{x}'_{\mathrm{S}};\boldsymbol{\theta}) = \frac{1}{2}\mathbf{x}'^{\top}_{\mathrm{S}}\,\mathbf{J}(\boldsymbol{\theta}')\,\mathbf{x}'_{\mathrm{S}}, \quad \boldsymbol{\theta} = \boldsymbol{\theta}' \cup \{\beta_k\}_{k=1}^{K}$$

Precision matrix (sparse, explicit) using only the first two terms

$$\mathbf{J}(\boldsymbol{\theta}') = \frac{1}{\lambda}\left\{\frac{\mathbf{I}}{N} + c_1\,\mathbf{J}_1(\boldsymbol{\theta}'')\right\}, \; \boldsymbol{\theta}'' = (\mu_s, \mu_t, K_t, K_s)^{\top}$$

Gradient Precision sub-matrix based on the normalized-weight matrix

$$[\mathbf{J}_1(\mathbf{h}_s,\mathbf{h}_t)]_{i,j} = -u_{i,j}(\mathbf{h}_s,\mathbf{h}_t) - u_{j,i}(\mathbf{h}_s,\mathbf{h}_t) + \delta_{i,j}\sum_{k=1}^{N}\left[u_{i,k}(\mathbf{h}_s,\mathbf{h}_t) + u_{k,i}(\mathbf{h}_s,\mathbf{h}_t)\right]$$

Normalized kernel weights: $u_{i,j}(\mathbf{h}_s,\mathbf{h}_t) = [\mathbf{U}]_{i,j}$

SLI Mode Predictor for Interpolation of Missing Data

- Modified energy functional in the presence of an unknown value

$$\mathcal{H}(\mathbf{x}_{\mathrm{S}};\boldsymbol{\theta}) = \frac{1}{2}\begin{bmatrix} \mathbf{x}'^{\top}_{\mathrm{S}} & x'_p \end{bmatrix}\begin{bmatrix} \mathbf{J}_{S,S} & \mathbf{J}_{S,P} \\ \mathbf{J}_{P,S} & J_{p,p} \end{bmatrix}\begin{bmatrix} \mathbf{x}'_{\mathrm{S}} \\ x'_p \end{bmatrix}$$

- x_p is the value at the *prediction point*
- $\hat{x}_p = \arg\min_{x_p} \hat{\mathcal{H}}(\mathbf{x}_{\mathrm{S}}, x_p; \boldsymbol{\theta}^*)$.
- The predictor is a linear equation (reminiscent of GMRFs) that can be evaluated with $\mathcal{O}(N)$ computational time complexity:

Conditional mean | Conditional variance

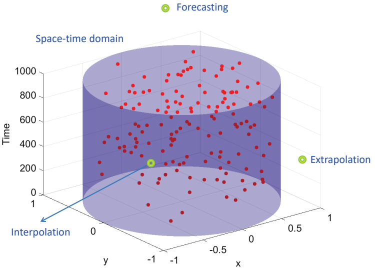
$$\hat{x}_p = m_{\mathrm{x}} - \frac{1}{J_{p,p}(\boldsymbol{\theta}'^*)}\sum_{i=1}^{N} J_{p,i}(\boldsymbol{\theta}'^*)\,(x_i - m_{\mathrm{x}}), \quad \sigma_p^2 = \frac{1}{J_{p,p}(\boldsymbol{\theta}'^*)}.$$

 [Hristopulos, 2015]

Space-Time data and parameter estimation

- Synthetic S-T data generated by the R package RandomFields (Schlather M, *et al.* (2019). RandomFields: Simulation and Analysis of Random Fields. R package version 3.3.6)
- ERA5 reanalysis data (ERA5 is the latest climate reanalysis produced by the European Centre for Medium-Range Weather Forecasts, providing hourly data on many atmospheric, land-surface and sea-state parameters together with estimates of uncertainty).

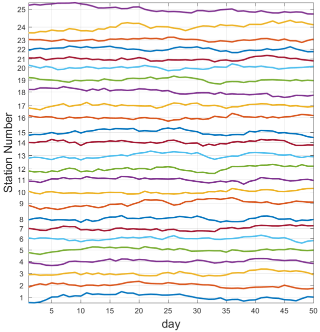
- Parameter vector: $\boldsymbol{\theta} = (\mu_s, K_s, \mu_t, K_t, \lambda, c_1, \beta_1, \ldots, \beta_K)^\top$
- K_s and K_t are pre-selected
- *Maximum Likelihood Estimation:* The log-determinant of the sparse precision matrix is calculated using LU decomposition

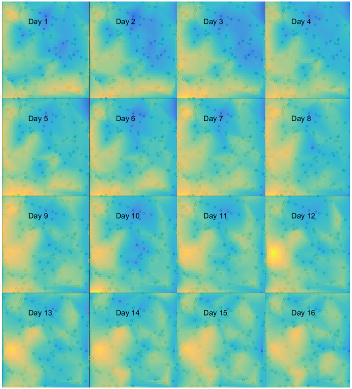


For more details see [Hristopulos & Agou, 2019].

Simulated S-T data from stationary random field

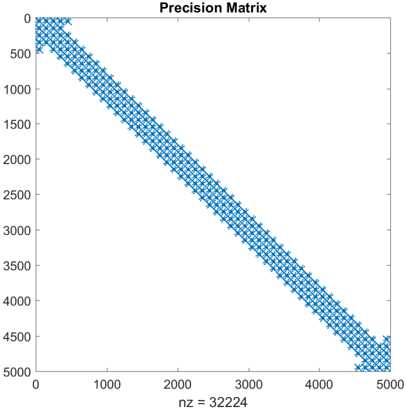
100 random locations and 50 time slices from a Gaussian RF with separable S-T exponential covariance

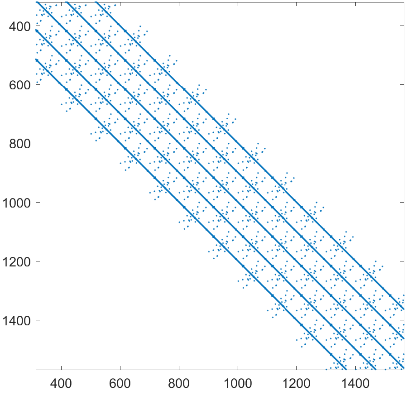




Simulated S-T data from stationary random field

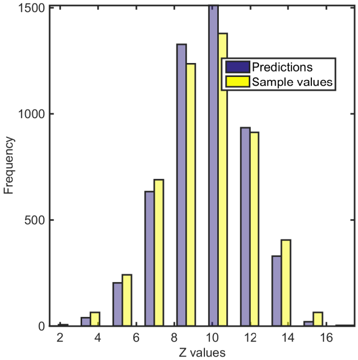
SLI Precision Matrix – Sparsity index ≈ 0.13%

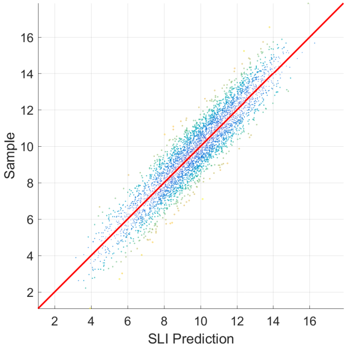




Simulated S-T data from stationary random field

Leave-one-time-slice-out Cross validation



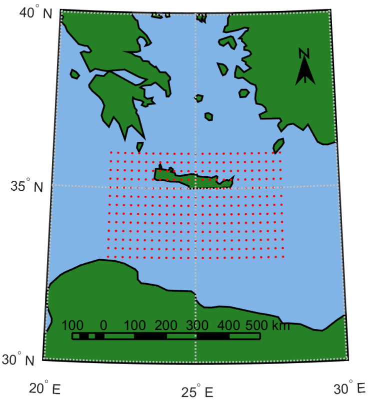


Reanalysis ERA5 Temperature data around Crete

Study design

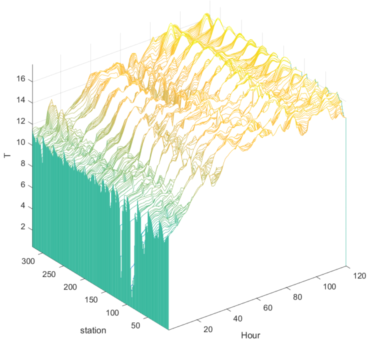
- Hourly temperature (degrees) for five days from 01-01-2017 00:00:00 to 05-01-2017 23:00:00
- Total of 39 000 data points
- SLI parameter estimation using MLE (quadratic kernel, ($K_s = K_t = 3$)
- Cross validation: Remove one time slice each time and predict using SLI

Spatial grid 13×25

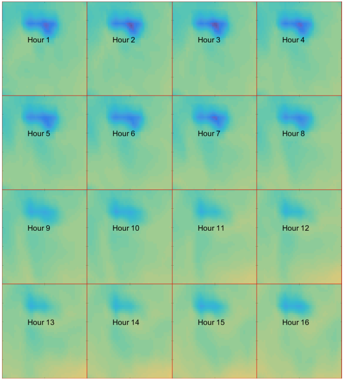


Reanalysis ERA5 Temperature data around Crete

Time series - all sites

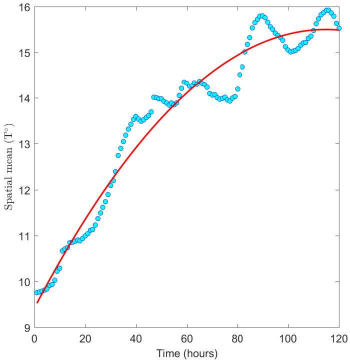


First few time slices



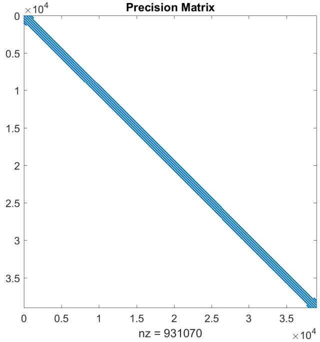
Reanalysis ERA5 Temperature data around Crete

Trend Modeling



$$m_x(t) = \beta_1 + \beta_2 t + \beta_3 t^2$$

Sparsity of SLI Precision Matrix



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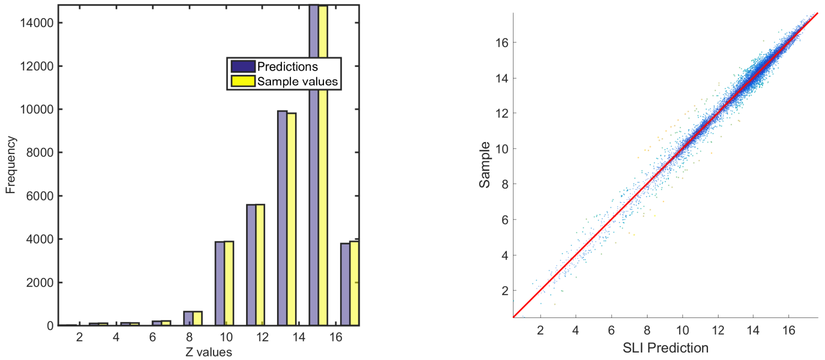

SLI precision matrix *sparsity index* $\approx$ 0.06%, i.e., $\approx$ 123 000 non-zero entries out of 1.521×10^9 matrix entries

Conclusions and Future Directions

- Statistical mechanics is a useful theoretical framework for developing local methods of S-T data analysis
- The stochastic local interaction model (SLI) extends GMRF ideas to scattered data without requiring the solution of an SPDE
- SLI employs compactly supported kernel functions with adaptive kernel bandwidths to construct an explicit precision matrix. This structure leads to semi-explicit prediction equations and *computationally efficient implementations*
- SLI prediction performance is comparable to Kriging (BLUE)

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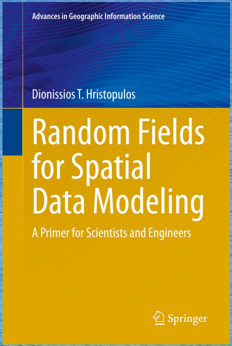

Random Fields for Spatial Data Modeling

For more information ...

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D. T. Hristopulos and S. Elogne (2007). Analytic properties and covariance functions of a new class of generalized Gibbs random fields. *IEEE Trans. Infor. Theory*, 53(12), 4667 - 4679.

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