





Statistical Learning for Spatial Data: Theory and Practice

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Natural phenomena:

- weather
- earthquakes
- rivers
- environment
- vegetation



Humanmade:

- urban planning
- · public services
- crimes
- agriculture

Spatial Data Characteristics

1. Spatial dependence structure



2. One single realization

Natural event



Deterioration of the environment



General Spatial Model

$$\mathbf{X} = \left\{ \mathbf{X}_{s}, s \in \mathcal{S} \right\}$$

Geostatistical Data:

- Observations: fixed, irregularly or regularly sampled
- Goal: modeling, prediction
- Example: hydrogeology (pH value)



Point Patterns:

- Observations: locations (and number n)
 are random
- Goal: capturing a pattern in data
- Example: seismology



Geostatistics: History and Applications

1950s: Danie G. Krige's study in mineral deposit (Krige, 1951)

1960s: Georges Matheron lays foundations of Geostatistics theory (Matheron, 1962)

Covariance function describes the dependence structure of data



Unknown in practice \Longrightarrow need to be **estimated**



Meteorology: weather patterns, climate trends, and atmospheric phenomena (Goovaerts, 2000)





Healthcare: spatial patterns of disease incidence and mortality (Oliver et al., 1998)

1970s: Temporal Hawkes Processes (HP) (Hawkes, 1971)

1980s: Introduction of HP to earthquake modeling (Ogata, 1988)

1990s: extension to spatio-temporal data: earthquakes exhibit both spatial and temporal clustering (Musmeci and Vere-Jones, 1992)



Seismology: mainshock-aftershock pattern (clustering and triggering) (Ogata, 1988; Daley and Vere-Jones, 2003)



Criminology: 'near-repeat victimization' pattern (Mohler et al., 2011; D'Angelo et al., 2022)



Epidemiology: spread of infectious diseases, patterns in disease occurrence (Meyer and Held, 2014; Kresin et al., 2022)

How to learn from spatial data that presents a dependence structure?

How does the dependence structure of the observed phenomenon affect the **performance** of the algorithms?

 \checkmark

GEOSTATISTICS

1. How **accurate** is the empirical covariance estimator?

2. What is the **non-asymptotic** performance of the Kriging predictor?



- 3. How to overcome the numerical and modeling challenges when learning from a spatiotemporal Hawkes process?
- 4. How to accurately model real-world situations?

A Statistical Learning View of Simple Kriging

Motivation

Machine Learning:

- Assets: statistical learning theory for independent data, non-parametric theory
- Limits: very few theoretical guarantees for spatial data

Spatial Analysis:

- Assets: take advantage of spatial structure (modelled by covariance function)
- Limits: very few non-parametric theories
- Limits: lack of non-asymptotic results for spatial data

Challenge 1: Provide statistical guarantees for **prediction**, under the form of **non-asymptotic** bounds, for **non-parametric** methods in the context of spatial data.



Notations

- $\mathcal{S} \subseteq \mathbb{R}^2$: spatial domain
- C(s, t) : covariance function

- $C(s,t) = Cov(\mathbf{X}_s, \mathbf{X}_t)$
- $X(s_d)$: observations of X $X(s_d) = (X_{s_i})_{1 \le i \le d}$ at locations $s_d = (s_i)_{1 \le i \le d}$.
- $c_d(s)$: covariance vector $c_d(s) = (Cov(X_s, X_{s_i}))_{1 < i < d}$
- $\Sigma(\mathbf{s}_d)$: covariance matrix $\Sigma(\mathbf{s}_d) = Var(\mathbf{X}(\mathbf{s}_d))$
- X': one single realization of X at locations $\sigma_n = (\sigma_i)_{1 \le i \le n}$.

 $\mathbf{X}'(\sigma_n) = \left(\mathbf{X}'_{\sigma_i}\right)_{1 \le i \le n}$

Simple Kriging Problem

Simple Kriging: predict the value of X at some unobserved location *s*, based on *d* sampled observations $(\mathbf{X}_{s_i})_{i \leq d}$, assuming a **linear** combination of the observations: $f_{\lambda}(s) = \langle \lambda(s), \mathbf{X}(\mathbf{s}_d) \rangle$, such that λ minimizes the variance.

$$f_{\lambda^*}(\mathbf{s}) = \ \mathbf{X}(\mathbf{s}_d)^{ op} \Sigma(\mathbf{s}_d)^{-1} \mathbf{c}_d(\mathbf{s})$$

 \hookrightarrow the weights λ^* depend on covariance function and s







→ <u>Motivation:</u> Need to establish rate bounds that assess the generalization capacity of the resulting predictive map

Accuracy of predictor: measured by the integrated Mean Squared Error (IMSE) over the spatial domain S:

$$\begin{split} L_{\mathcal{S}}(f_{\lambda}) &= \mathbb{E}_{\mathsf{X}} \left[\int_{s \in \mathcal{S}} \left(f_{\lambda}(s) - \mathsf{X}_{s} \right)^{2} ds \right] \\ &= \int_{s \in \mathcal{S}} \left(\mathsf{Var}(\mathsf{X}_{s}) + \ \lambda(s)^{\top} \Sigma(\mathsf{s}_{d}) \lambda(s) - 2 \, \mathsf{c}_{d}(s)^{\top} \lambda(s) \right) ds \end{split}$$

Statistical guarantees of predictor: The global excess risk quantifies the gap between the optimal theoretical predictor and the empirical predictor errors:

$$L_{\mathcal{S}}(f_{\widehat{\lambda}}) - L_{\mathcal{S}}(f_{\lambda^*}) = \mathbb{E}_{X}\left[\int_{s \in \mathcal{S}} \left(f_{\widehat{\lambda}}(s) - f_{\lambda^*}(s)\right)^2 ds\right]$$

Limitation: unique realisation for learning with only n observations

Assumption 1: X second order stationary with isotropic covariance (Cressie, 1993): constant mean $\mu \in \mathbb{R}$, and invariant covariance C (depends only on distance h):

$$\exists c, C(s,t) = c(\|t-s\|) = c(h)$$

 $\longrightarrow \sqrt{\text{Solution: X}}$ is sufficiently homogeneous inside the spatial domain (its characteristics are identical from one point to another)

Assumptions (suite)

• Assumption 2: X Gaussian random field with zero mean and positive definite covariance function

 $\longrightarrow \sqrt{\text{strict stationarity, all laws}}$ are known, Bochner's theorem (Stein, 1999; Hall and Patil, 1994)

• Assumption 3: In-fill asymptotic: number of observations within spatial domain S increases (denser and denser grid) and regular grid (Cressie, 1993)

 $\longrightarrow \sqrt{\text{accurate}}$ and **unbiased** estimator

Estimation of the Dependence Structure

How accurate is the empirical covariance estimator?

How data points are related to each other, based on their spatial proximity?

 $\longrightarrow {\bf covariance}$ and ${\bf semi-variogram}$ functions describe how the spatial correlation between data points changes with distance

Covariance:

Semi-variogram:

$$c(h) = \mathbb{E}\left[\left(\mathbf{X}_{s+h} - \mu \right) \left(\mathbf{X}_{s} - \mu \right) \right] \qquad \gamma(h) = \frac{1}{2} \mathbb{E}\left[\left(\mathbf{X}_{s+h} - \mathbf{X}_{s} \right)^{2} \right]$$

Property: For all $h \in \mathbb{R}$, $\gamma(h) = c(0) - c(h)$.

Non-parametric Estimation of the Dependence Structure

Empirical semi-variogram (Matheron, 1962):

$$\widehat{\gamma}(h) = \frac{1}{2n_h} \sum_{(s_i, s_j) \in N(h)} \left(\mathbf{X}_{s_i} - \mathbf{X}_{s_j} \right)^2,$$

where N(h) is the set of pairs of sites at a distance h (set of neighbors) and n_h its cardinality.

Advantages:

- flexible approach to the massive character of spatial datasets
- does not require knowledge of mean
- unbiased estimator (for regular grids)
- under Gaussianity assumption, $\hat{\gamma}(h)$ is sum of **independent** χ^2 variables

Additional Assumptions



• Assumption 4: $\exists \theta, \forall h \ge \theta, c(h) = 0$ (border hypothesis)

• Assumption 5: c is of class C¹ and its gradient is bounded by Q (regularity/smoothness hypothesis)

 \longrightarrow \checkmark for the estimation error at all lags

Corollary (Siviero et al., 2023)

Suppose that Assumptions 1–5 are satisfied. Then, for any $\delta \in (0, 1)$, we have with probability at least $1 - \delta$:

$$\sup_{h\geq 0} \left|\widehat{c}(h) - c(h)\right| \leq C_3 \sqrt{\log(4n/\delta)/n} + Q/(\sqrt{n}-1),$$

as soon as $n \ge C'_3 \log(4n/\delta)$, where C_3 and C'_3 are positive constants depending on θ and on the bounds of the eigenvalues of the covariance matrix solely.

• **Distribution of** $\widehat{\gamma}(h)$: Under the Gaussian assumption (Hyp 2),



where $\ell_i(h)$'s are the eigenvalues of $L(n,h)\Sigma(\sigma_n)$.

• **Poisson tail bounds:** Thanks to recent results in (Bercu et al., 2015) and (Wang and Ma, 2020):

$$\mathbb{P}\left(\left|\widehat{\gamma}(h)-\gamma(h)\right|\geq t\right)\leq e^{-C_{1}nt}+e^{-C_{1}'nt^{2}},$$

where C_1 and C'_1 are positive constants depending on θ (Hyp 4).

• Estimation for all lags: Thanks to a piece-wise constant estimator and the regularity assumption (Hyp 5).

Statistical Learning Guarantees for the Kriging Method

What are the **non-asymptotic guarantees** for the Kriging predictor?

Statistical Learning Theory

ERM: $f_{\hat{\lambda}}$ is the empirical risk minimizer of

$$\widehat{L}_{\mathcal{S}}(f_{\lambda}) = \int_{s \in \mathcal{S}} \left(\widehat{c}(0) + \lambda(s)^{\top} \widehat{\Sigma}(\mathbf{s}_{d}) \lambda(s) - 2 \, \widehat{\mathbf{c}}_{d}(s)^{\top} \lambda(s) \right) ds$$

<u>GOAL:</u> define **non-asymptotic** bound of global excess risk:

$$\begin{split} L_{\mathcal{S}}(f_{\widehat{\lambda}}) - L_{\mathcal{S}}(f_{\lambda^*}) &= \\ \int_{s \in \mathcal{S}} \left(\widehat{\lambda}(s) - \lambda^*(s) \right)^\top \Sigma(\mathbf{s}_d) \widehat{\lambda}(s) + \lambda^*(s)^\top \Sigma(\mathbf{s}_d) \left(\widehat{\lambda}(s) - \lambda^*(s) \right) \\ &- 2 \mathbf{c}_d(s)^\top \left(\widehat{\lambda}(s) - \lambda^*(s) \right) ds \end{split}$$

Theorem (Siviero et al., 2023)

Suppose that Assumptions 1–5 are satisfied. Then, for any $\delta \in (0, 1)$, we have with probability at least $1 - \delta$:

$$L_{\mathcal{S}}(f_{\widehat{\Lambda}_d}) - L_{\mathcal{S}}(f_{\lambda^*}) \leq C_6 \, d^2 \, \sqrt{\log(4n/\delta)/n} + C_6' \, d^2 \, Q/(\sqrt{n}-1),$$

as soon as $n \ge C_6'' \log(4n/\delta)$, where C_6 , C_6' and C_6'' are positive constants depending on θ and on the bounds of the eigenvalues of the covariance matrix solely.

$$\begin{split} \sup_{s \in \mathcal{S}} ||\widehat{\lambda}(s) - \lambda^*(s)|| &\leq \underbrace{|||\Sigma(\mathbf{s}_d)^{-1}|||}_{s \in \mathcal{S}} \underbrace{\sup_{s \in \mathcal{S}} ||\widehat{\mathbf{c}}_d(s) - \mathbf{c}_d(s)||}_{s \in \mathcal{S}} \\ &+ \underbrace{|||\widehat{\Sigma}(\mathbf{s}_d)^{-1} - \Sigma(\mathbf{s}_d)^{-1}|||}_{N_3} \underbrace{\sup_{s \in \mathcal{S}} ||\widehat{\mathbf{c}}_d(s)||}_{s \in \mathcal{A}}, \end{split}$$

where

- N_1 : From bounds on eigenvalues of $\Sigma(\mathbf{s}_d)$
- N₂: From Corollary
- N₃: Non-asymptotic bound on the accuracy of the precision matrix estimation
- N₄: From Corollary and Assumption 5

Illustrative Experiments

Averaged MSE on 100 realisations, with two covariance models, for varying θ



 $\longrightarrow \checkmark$ experiments **corroborate** our theoretical results: the error depends on θ (role of technical assumptions is verified) $\longrightarrow \checkmark$ results for Gaussian covariance encourages to **relax Hyp 4**

Contributions

1. Flexible covariance estimation:

We develop **tail bounds** for the **non-parametric** covariance estimator.

2. Statistical guarantees for Kriging:

We develop a novel theoretical framework offering **guarantees** for empirical Kriging rules in the form of **non-asymptotic bounds**.

 Our numerical experiments on simulated and real meteorological data corroborate our theoretical results. GitHub: github.com/EmiliaSiv/Simple-Kriging-Code

Flexible Parametric Inference for Space-Time Hawkes Processes

Motivation

Seismology

 Mainshock-aftershock clustering behavior



• (Vere-Jones, 1970; Ogata, 1988)

Criminology

 Near-repeat victimization pattern



• (Mohler, 2014; Zhu and Xie, 2022)

Challenge 2: Develop a new, efficient, and accurate method to predict from spatio-temporal data, such that it is flexible in modeling real-world situations.

Hawkes Processes

- Point process: collection of events, randomly distributed over time or space
 - \hookrightarrow behavior characterized by conditional intensity function.
- Hawkes (or self-exciting) process: each event increases the likelihood of future events in its neighborhood
 - \hookrightarrow intensity depends on time, location, and history of the process.



Figure: Univariate spatiotemporal point process

Conditional Intensity Function



Notations

Given $D \ge 1$ type of events, for each $i \in \{1, \dots, D\}$, the intensity function of the *i*-th process of a multivariate spatio-temporal Hawkes process (MSTHP):



- + $\ensuremath{ T \in \mathbb{R}_+ :}$ stopping time, $\mathcal{S} \subset \mathbb{R}^2 :$ compact set of the space domain
- μ_i : parameter controlling spontaneous event apparition rate with $\mu_i > 0$
- \mathcal{H}_{t}^{i} : collection of past events $u_{n}^{i} = (x_{n}^{i}, y_{n}^{i}, t_{n}^{i}), (x_{n}^{i}, y_{n}^{i}) \in \mathcal{S}, t_{n}^{i} \in [0, t]$
- + $lpha_{ij}$: describes excitation behavior between events with 0 $\leq lpha_{ij} <$ 1
- $g_{ij} : S \times [0, T] \mapsto \mathbb{R}_+$: spatio-temporal *kernel* (excitation function): influence of past events onto future events

$$\longrightarrow$$
 parameters: $oldsymbol{ heta}=\{oldsymbol{\mu}_{i},oldsymbol{lpha}_{ij},oldsymbol{\eta}_{ij}\}_{ij}$

Two assumptions are commonly made:

- Space-time separability (Mohler, 2014; Ilhan and Kozat, 2020)
 √ brings simplicity
 × not realistic (space-time interactions)
- Constrained kernel models (Chen et al., 2021)
 - $\sqrt{}$ computational efficiency
 - \times **restrictive** for some real-world situations
- Motivation: Need to develop a parametric method allowing (1) any kind of kernels and (2) space-time interactions

Flexible Inference Approach for MSTHP

How to accurately model real-world situations using MSTHP?

Inspired by recent work of (Staerman et al., 2023), the inference approach relies on **three key components**:

 <u>Discretization</u>: define a three dimensional regular grid G = G_S × G_T with Δ_S, Δ_T > 0 the stepsizes of the spatial and temporal grids, project the observed events on these grids and define Hⁱ_T.

 $\hookrightarrow \sqrt{}$ we can rewrite the **intensity in a discretized manner** $\tilde{\lambda}$.

2. <u>Finite-support Kernels</u>: consider the spatio-temporal kernels to be of finite lengths W_S and W_T , and define $L_T = \lfloor W_T / \Delta_T \rfloor + 1$, $L_S = \lfloor 2W_S / \Delta_S \rfloor + 1$ the number of points on the discretized temporal and spatial support.

 $\hookrightarrow \sqrt{\text{reduce computational burden}}.$

- 3. <u>Precomputations:</u> in the loss, terms appear that do not depend on the set of parameters θ :
 - P_1 : $\Phi_j(\tau; G)$
 - P_2 : $\Phi_j(\tau; \widetilde{\mathcal{H}}_T^i)$
 - **P**₃: $\Psi_{j,k}(\tau, \tau'; G)$

 $\hookrightarrow \sqrt{}$ these terms can be **precomputed** at initialization and used at each step of the optimization procedure.

 \implies Gradient-based optimization: approach efficiently computes exact gradients for each parameter

Table 1: Negative Log Likelihood (NLL) values on test sets of various extracted earthquake datasets (NCEDC, nce, 2014) with several triggering (separable and non-separable) kernels. The best NLL is in **bold** and the second best is <u>underlined</u>.

Setting	1987 - 1989	2003 - 2014	1967 - 2003	
TG + TG	2.77	1.76	0.72	
TG + EXP	3.25 2.14		0.65	
TG + KUM	2.98	2.66	0.57	
POW + TG	2.11	1.04	0.18	
POW + EXP	1.72 1.57		<u>0.20</u>	
POW + KUM	<u>2.06</u>	<u>1.50</u>	0.29	
NS1 ¹	3.77	2.68	0.88	
NS2 ²	3.77	2.67	0.87	

¹ Function from the class of non-separable functions in (Cressie and Huang, 1999)

² Spatio-temporal function from the (Gneiting, 2002) class

Table 2: NLL values on test sets of various extracted burglary datasets of theChicago Crime Dataset with several triggering (separable and non-separable)kernels.

Setting	2008	2002 - 2004	2002 - 2006	
TG + TG	-0.24	0.26	0.51	
TG + EXP	-0.24	0.38	0.60	
TG + KUM	-0.23	0.35	0.54	
POW + TG	0.54	1.04	1.10	
POW + EXP	1.27	1.03	1.08	
POW + KUM	0.83	0.86	0.91	
NS1	<u>-0.37</u>	<u>-0.43</u>	<u>-0.28</u>	
NS2	-0.95	-0.49	-0.31	

Table 3: Spatial and Temporal NLL values on test sets of various extracted real-world datasets.

Dataset	Earthquake		COVID-19		Citybike	
Models	Spatial	Temporal	Spatial	Temporal	Spatial	Temporal
NSTPP ¹	0.886	-0.623	1.9	-2.25	2.38	-1.09
DeepSTPP ²	4.92	-0.174	0.361	-1.09	-4.94	-1.13
DSTPP ³	<u>0.413</u>	<u>-1.1</u>	<u>0.35</u>	<u>-2.66</u>	0.529	<u>-2.43</u>
Our approach	-0.501	-10.021	-0.887	-6.336	0.083	-4.275

¹ NSTPP from (Chen et al., 2021)

² DeppSTPP from (Zhou et al., 2022)

³ DSTPP from(Yuan et al., 2023)

Contributions

 We develop an efficient and flexible method for estimating STHP model parameters allowing (1) any (separable) parametric kernel, and (2) space-time non-separable kernels

 $\longrightarrow \sqrt{}$ our method **enhances precision and adaptibility** when dealing with complex dependencies in real data.

2. Our numerical experiments on simulated and real data show flexibility, adaptability to phenomenon's characteristics, and accuracy compared to SOTA.

 $\longrightarrow GitHub: {\tt github.com/EmiliaSiv/}$

Flexible-Parametric-Inference-for-Space-Time-Hawkes-Processes

Perspectives

- Gradually relax some hypotheses:
 - Assumption 2 (stationary hypothesis): locally stationary processes
 - Assumption 4 (border hypothesis) less restrictive: $c(h) \searrow 0$
 - Assumption 5 (regularity hypothesis): other smoothing techniques
 - $\rightarrow \sqrt{\text{extend}}$ our main results to a more general framework
- **Irregular grid**: define different sets of neighbors, difficulties when controlling the spectrum of the covariance matrix

 $\longrightarrow \surd$ cover more real-world situations

- Non-constant baseline and irregular discretization grid
 → √ improve accuracy, based on additional information on
 phenomenon's characteristics
- Marked spatio-temporal Hawkes processes:

 $\lambda_i(x, y, t, M | \mathcal{H}_t) = \mu_i + \sum_{j=1}^{D} \sum_{u_n^j \in \mathcal{H}_t^j} \alpha_{ij} g_{ij}(x - x_n^j, y - y_n^j, t - t_n^j, M - M_n^j),$

where M_n^j is the mark of the event

 $\longrightarrow \sqrt{}$ additional important features (magnitude of an earthquake, type of crime, etc)

• Non-separability in marked processes

 $\longrightarrow \sqrt{}$ accounting for space-time and marks interactions

• Python library with MIND team (Inria)

Work in progress: Hydrogeology and Spatial Analysis, with Juan Guzmán

Publications:

E. Siviero, E. Chautru, & S. Clémençon (2023).
 A Statistical Learning View of Simple Kriging. TEST, 33(1), 271-296.

E. Siviero, G. Staerman, S. Clémençon, & T. Moreau (2024).
 Flexible Parametric Inference for Space-Time Hawkes Processes. ArXiv preprint arXiv:2406.06849 (Submitted).

Presentations:

- CAp 2022 (poster), COMPSTAT 2022 (oral)
 - MIND team Seminar 2023 (oral), COMPSTAT 2024 (oral)

GitHub:

- github.com/EmiliaSiv/Simple-Kriging-Code
- github.com/EmiliaSiv/
 - Flexible-Parametric-Inference-for-Space-Time-Hawkes-Processes

Thanks for your attention !

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