When are linear predictions of random fields using wrong mean and covariance functions asymptotically optimal?

Kristin Kirchner

Joint work with David Bolin (KAUST)

One World Seminar: Stochastic Numerics and Inverse Problems

March 2, 2022



Linear spatial prediction



Consider a random field $\{Z(x) : x \in \mathcal{X}\}$ on a compact metric space \mathcal{X} .

Aim: Predict its value $Z(x^*)$ at $x^* \in \mathcal{X}$ based on a set of observations $\{Z(x_j)\}_{j=1}^n$ for locations $x_1, \ldots, x_n \in \mathcal{X}$ all distinct from x^* .

The kriging predictor is the linear predictor

$$Z_n(x^*) = \alpha_0 + \sum_{j=1}^n \alpha_j Z(x_j)$$

based on the observations, where $\alpha_0, \ldots, \alpha_n \in \mathbb{R}$ are chosen such that the variance of the error $Z_n(x^*) - Z(x^*)$ is minimized.

ŤUDelft

Model misspecification

If $m(\cdot)$ and $\varrho(\cdot, \cdot)$ are the mean and the covariance function of Z, then

$$Z_n(x^*) = m(x^*) + \mathbf{c}^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{Z} - \mathbf{m}), \qquad (*)$$

where

$$\mathbf{c} \coloneqq (\varrho(x^*, x_1), \dots, \varrho(x^*, x_n))^\top, \qquad \mathbf{\Sigma}_{ij} \coloneqq \varrho(x_i, x_j), \\ \mathbf{Z} \coloneqq (Z(x_1), \dots, Z(x_n))^\top, \qquad \mathbf{m} \coloneqq (m(x_1), \dots, m(x_n))^\top.$$

 \Rightarrow the kriging predictor depends only on (m, ϱ) .

Therefore, from now on we assume that $Z \sim \mu = N(m, \varrho)$.

We are interested in the asymptotic behavior of

$$\frac{\mathsf{E}\big[(\widetilde{Z}_n(x^*) - Z(x^*))^2\big]}{\mathsf{E}\big[(Z_n(x^*) - Z(x^*))^2\big]} \quad \text{as} \quad n \to \infty,$$

where the linear predictor $\widetilde{Z}_n(x^*)$ is computed using (*) with $(\widetilde{m}, \widetilde{\varrho})$.

TUDelft

What was known?

• M. L. Stein¹ showed that the best linear predictor based on $(\widetilde{m}, \widetilde{\varrho})$ is asymptotically optimal, as $n \to \infty$, provided that

 $\mu = N(m, \varrho)$ and $\widetilde{\mu} = N(\widetilde{m}, \widetilde{\varrho})$ are equivalent.

- This result in fact holds *uniformly* with respect to x* and, moreover, uniformly for each linear functional φ such that φ(Z) has finite variance².
- Less restrictive conditions have been derived for some specific cases, such as *periodic* fields³ on [0,1]^d and *stationary* fields⁴ on ℝ^d, i.e. *ρ*(*x*, *y*) = *ρ*(*x* − *y*), observed on a lattice.

 $^{^{1}}$ M. L. Stein (1988). "Asymptotically efficient prediction of a random field with a misspecified covariance function". In: *Ann. Stat.* 16.1, pp. 55–63

²M. L. Stein (1990). "Uniform asymptotic optimality of linear predictions of a random field using an incorrect second-order structure". In: *Ann. Stat.* 18.2, pp. 850–872

³M. L. Stein (1997). "Efficiency of linear predictors for periodic processes using an incorrect covariance function". In: J. Statist. Plann. Inference 58.2, pp. 321–331

⁴M. L. Stein (1999). "Predicting random fields with increasing dense observations". In: Ann. Appl. Probab. 9.1, pp. 242–273

Goals of our work

For any constant $c \in (0, \infty)$, the linear predictor based on $(m, c\varrho)$ is equal to that based on (m, ϱ) , whereas

 $\forall c \neq 1: \quad \mu = \mathsf{N}(m, \varrho) \perp \widetilde{\mu} = \mathsf{N}(m, c\varrho).$

 \Rightarrow Equivalence of the measures μ and $\tilde{\mu}$ is a *sufficient, but not necessary* assumption for asymptotic optimality of linear predictions.

Topics of this talk

- necessary and sufficient conditions on (*m̃*, *ṽ*) for uniform asymptotic optimality of linear predictions;
- 2 explicit conditions for a large class of non-stationary models and
 - equivalence of Gaussian measures;
 - asymptotic optimality of linear predictions.

Necessary and sufficient conditions for asymptotic optimality Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis Generalized Whittle–Matérn fields Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Necessary and sufficient conditions for asymptotic optimality Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis Generalized Whittle–Matérn fields Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Setting

 Z: X × Ω → ℝ is a square-integrable Gaussian stochastic process indexed by a connected, compact metric space (X, d_X), with strictly positive and finite Borel measure ν_X : B(X) → [0,∞).

Notation : $L_2 \coloneqq L_2(\mathcal{X}, \mathcal{B}(\mathcal{X}), \nu_{\mathcal{X}}).$

Z has mean m ∈ L₂, strictly positive definite and continuous covariance function ρ: X × X → ℝ, and covariance operator

$$\mathcal{C}: L_2 \to L_2, \qquad (\mathcal{C}w)(x) \coloneqq \int_{\mathcal{X}} \varrho(x, x') w(x') \, \mathrm{d}\nu_{\mathcal{X}}(x').$$

C is self-adjoint, positive definite, and trace-class on L_2 .

 We write μ = N(m,C) for the Gaussian measure on L₂ induced by the process Z, i.e., for every Borel set A ∈ B(L₂),

$$\mu(A) = \mathbb{P}(\{\omega \in \Omega : Z(\cdot, \omega) \in A\}).$$



Kriging predictor as orthogonal projection

- $Z^0 := Z m$ is a *centered* Gaussian process.
- The vector space $\mathbb{Z}^0 \subset L_2(\Omega, \mathbb{P})$ contains finite linear combinations

 $\mathcal{Z}^{0} := \left\{ \sum_{j=1}^{K} \alpha_{j} Z^{0}(x_{j}) : K \in \mathbb{N}, \ \alpha_{j} \in \mathbb{R}, \ x_{j} \in \mathcal{X} \right\}, \quad \mathcal{H}^{0} := \overline{\mathcal{Z}^{0}}^{\|\cdot\|_{L_{2}(\Omega, \mathbb{P})}}.$

• Every $h = \sum_{j \le K} \alpha_j Z(x_j)$ has a representation

 $h = c + h^0$, with $c \in \mathbb{R}$, $h^0 \in \mathcal{Z}^0 \subset \mathcal{H}^0$.

We thus define the Hilbert space $\mathcal{H} \coloneqq \mathbb{R} \oplus \mathcal{H}^0$,

 $(g,h)_{\mathcal{H}} = \mathsf{E}[g]\mathsf{E}[h] + (g - \mathsf{E}[g], h - \mathsf{E}[h])_{\mathcal{H}^0} = \mathsf{E}[gh].$

 The kriging predictor h_n of h ∈ H based on H_n := ℝ ⊕ H⁰_n ⊂ ℝ ⊕ H⁰ is the H-orthogonal projection of h onto H_n:

$$h_n \in \mathcal{H}_n: \quad (h_n - h, g_n)_{\mathcal{H}} = \mathsf{E}\left[(h_n - h)g_n\right] = 0 \qquad \forall g_n \in \mathcal{H}_n,$$

$$h_n \in \mathcal{H}_n: \quad \mathsf{E}\left[(h_n - h)^2\right] = \inf_{g_n \in \mathcal{H}_n} \mathsf{E}\left[(g_n - h)^2\right].$$



Problem formulation

$$h_n \in \mathcal{H}_n$$
: $(h_n - h, g_n)_{\mathcal{H}} = \mathsf{E}[(h_n - h)g_n] = 0 \qquad \forall g_n \in \mathcal{H}_n,$

Main question

What happens if, instead of h_n , we use the linear predictor \tilde{h}_n which is the kriging predictor if $\tilde{\mu} = N(\tilde{m}, \tilde{C})$ was the correct model?

"Computing orthogonal projections with the wrong inner product"



Consistent kriging prediction

We require that, for every h ∈ H, the corresponding kriging predictors {h_n}_{n∈N} are consistent in the sense that

$$\lim_{n\to\infty} \mathsf{E}\big[(h_n-h)^2\big] = \lim_{n\to\infty} \|h_n-h\|_{\mathcal{H}}^2 = 0. \qquad (density)$$

• Let S^{μ}_{adm} contain all *admissible* sequences $\{\mathcal{H}_n\}_{n\in\mathbb{N}}$ of subspaces $\mathcal{H}_n \subset \mathcal{H}$ which provide μ -consistent kriging prediction,

$$S_{adm}^{\mu} \coloneqq \left\{ \{\mathcal{H}_n\}_{n \in \mathbb{N}} \mid \forall n \in \mathbb{N} : \mathcal{H}_n = \mathbb{R} \oplus \mathcal{H}_n^0 \text{ with } \dim(\mathcal{H}_n^0) = n, \\ \forall h \in \mathcal{H} : \{h_n\}_{n \in \mathbb{N}} \text{ satisfy } (density) \right\}.$$

Example

Suppose that m, ϱ are continuous and that every \mathcal{H}_n is generated by point observations $Z(x_1), Z(x_2), \ldots$ Then, $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in S^{\mu}_{adm}$ if $\{x_j\}_{j \in \mathbb{N}}$ is a sequence in $(\mathcal{X}, d_{\mathcal{X}})$ which accumulates at any $x^* \in \mathcal{X}$.

ŤUDelft

Necessary and sufficient conditions for asymptotic optimality Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on ℝ^d
 Common eigenbasis
 Generalized Whittle–Matérn fields
 Isomorphic Cameron–Martin spaces
 Equivalence of measures and asymptotically optimal linear prediction
 Summary and simulations

Main assumptions

The Assumptions

Let $\varrho, \tilde{\varrho}: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be two continuous, (strictly) positive definite covariance functions. Assume that the corresponding covariance operators $\mathcal{C}, \tilde{\mathcal{C}}: L_2 \to L_2$, and $m, \tilde{m} \in L_2$ are such that:

I. The vector spaces

 $\mathcal{C}^{1/2}(L_2), \ \left(\mathcal{C}^{-1/2} \cdot, \mathcal{C}^{-1/2} \cdot\right)_{L_2} \quad \text{and} \quad \widetilde{\mathcal{C}}^{1/2}(L_2), \ \left(\widetilde{\mathcal{C}}^{-1/2} \cdot, \widetilde{\mathcal{C}}^{-1/2} \cdot\right)_{L_2}$

are norm equivalent Hilbert spaces.

- II. The difference of the means satisfies $m \widetilde{m} \in C^{1/2}(L_2)$.
- III. There exists a positive constant $a \in (0, \infty)$ such that the operator

$$T_a: L_2 \to L_2, \qquad T_a:= \mathcal{C}^{-1/2}\widetilde{\mathcal{C}}\mathcal{C}^{-1/2} - a\mathcal{I}$$

is *compact* on L_2 . Here \mathcal{I} denotes the identity on L_2 .



Theorem (Asymptotic optimality, K. and Bolin, 2020)

Let $\mu = N(m, C)$ and $\tilde{\mu} = N(\tilde{m}, \tilde{C})$. Let h_n, \tilde{h}_n denote the best linear predictors of h based on \mathcal{H}_n and μ resp. $\tilde{\mu}$. Then, any of the assertions,

$$\lim_{n \to \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\mathbb{E}\left[(\widetilde{h}_n - h)^2\right]}{\mathbb{E}\left[(h_n - h)^2\right]} = 1,$$
$$\lim_{n \to \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\widetilde{\mathbb{E}}\left[(h_n - h)^2\right]}{\widetilde{\mathbb{E}}\left[(\widetilde{h}_n - h)^2\right]} = 1,$$
$$\lim_{h \to \infty} \sup_{h \in \mathcal{H}_{-n}} \left|\frac{\widetilde{\mathbb{E}}\left[(h_n - h)^2\right]}{\mathbb{E}\left[(h_n - h)^2\right]} - a\right| = 0,$$
$$\lim_{h \in \mathcal{H}_{-n}} \sup_{h \in \mathcal{H}_{-n}} \left|\frac{\mathbb{E}\left[(\widetilde{h}_n - h)^2\right]}{\widetilde{\mathbb{E}}\left[(\widetilde{h}_n - h)^2\right]} - \frac{1}{a}\right| = 0,$$

holds for all $\{\mathcal{H}_n\}_{n\in\mathbb{N}} \in S_{adm}^{\mu}$ if and only if the Assumptions I–III are satisfied. The constant $a \in (0, \infty)$ is the same as that in Assumption III.

Comparison with the Feldman-Hájek theorem

Equivalence of Gaussian measures

Let μ and $\widetilde{\mu}$ be two measures on $(L_2, \mathcal{B}(L_2))$. Then, μ and $\widetilde{\mu}$ are called

- equivalent if $\mu(A) = 0 \Leftrightarrow \widetilde{\mu}(A) = 0$;
- orthogonal if there exists $B \in \mathcal{B}(L_2)$ with $\mu(B) = 0$ and $\tilde{\mu}(B) = 1$.

Theorem (Feldman–Hájek)

Two Gaussian measures $\mu = N(m, C)$ and $\tilde{\mu} = N(\tilde{m}, \tilde{C})$ on a separable Hilbert space $(E, (\cdot, \cdot)_E)$ are either orthogonal or equivalent. They are equivalent if and only if the following conditions are satisfied:

- The Cameron–Martin spaces $C^{1/2}(E)$, $\widetilde{C}^{1/2}(E)$ are norm equivalent.
- The difference of the means satisfies $m \widetilde{m} \in \mathcal{C}^{1/2}(E)$.
- The operator $T_1 := C^{-1/2} \widetilde{C} C^{-1/2} Id_E$ is Hilbert–Schmidt on E.

Proposition (Role of Assumption I)

Let $\mu = N(m, C)$, $\tilde{\mu} = N(\tilde{m}, \tilde{C})$, and define $\mathcal{H}^0, \tilde{\mathcal{H}}^0$ with respect to the measures μ and $\tilde{\mu}$, respectively. The following are equivalent:

- (i) Assumption I is satisfied.
- (ii) The linear operator $\widetilde{C}^{1/2}C^{-1/2}: L_2 \to L_2$ is an isomorphism.
- (iii) The Hilbert spaces $\mathcal{H}^0, \widetilde{\mathcal{H}}^0$ are norm equivalent. In particular,

 $\exists k_0, k_1 > 0: \quad k_0 \operatorname{Var}[h] \leq \widetilde{\operatorname{Var}}[h] \leq k_1 \operatorname{Var}[h] \quad \forall h \in \mathcal{H}.$

(iv) There exist $0 < k \le K < \infty$ such that, for every $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{adm}^{\mu}$, for all $n \in \mathbb{N}$, and every $h \in \mathcal{H}_{-n}$,

 $\frac{\widetilde{\operatorname{Var}}[h_n-h]}{\operatorname{Var}[h_n-h]}, \ \frac{\operatorname{Var}[\widetilde{h}_n-h]}{\widetilde{\operatorname{Var}}[\widetilde{h}_n-h]}, \ \frac{\operatorname{Var}[\widetilde{h}_n-h]}{\operatorname{Var}[h_n-h]}, \ \frac{\widetilde{\operatorname{Var}}[h_n-h]}{\widetilde{\operatorname{Var}}[\widetilde{h}_n-h]} \in [k,K].$

 h_n, \tilde{h}_n are the best linear predictors of h based on \mathcal{H}_n and μ resp. $\tilde{\mu}$.



Proposition (Role of Assumptions I and III)

Let $\mu = N(m, C)$ and $\tilde{\mu} = N(\tilde{m}, \tilde{C})$. Let h_n, \tilde{h}_n denote the best linear predictors of h based on \mathcal{H}_n and μ resp. $\tilde{\mu}$. Then, any of the assertions,

$$\lim_{n \to \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\operatorname{Var}[\overline{h}_n - h]}{\operatorname{Var}[h_n - h]} = 1,$$
$$\lim_{n \to \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\widetilde{\operatorname{Var}}[h_n - h]}{\widetilde{\operatorname{Var}}[\overline{h}_n - h]} = 1,$$
$$\lim_{h \to \infty} \sup_{h \in \mathcal{H}_{-n}} \left| \frac{\widetilde{\operatorname{Var}}[h_n - h]}{\operatorname{Var}[h_n - h]} - a \right| = 0,$$
$$\lim_{n \to \infty} \sup_{h \in \mathcal{H}_{-n}} \left| \frac{\operatorname{Var}[\widetilde{h}_n - h]}{\widetilde{\operatorname{Var}}[\widetilde{h}_n - h]} - \frac{1}{a} \right| = 0,$$

holds for all $\{\mathcal{H}_n\}_{n\in\mathbb{N}} \in S_{adm}^{\mu}$ if and only if Assumptions I and III are fulfilled. The constant $a \in (0, \infty)$ is the same as that in Assumption III.

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d

Common eigenbasis Generalized Whittle–Matérn fields Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Examples of valid covariance models and metric spaces

Valid covariance functions are given by the Matérn class,

$$\varrho(x,x') \coloneqq \varrho_0(d_{\mathcal{X}}(x,x')), \qquad \varrho_0(r) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)} (\kappa r)^{\nu} \mathcal{K}_{\nu}(\kappa r), \quad r \ge 0,$$

on the compact metric space $(\mathcal{X}, d_{\mathcal{X}})$, where

- $\mathcal{X} \subset \mathbb{R}^d$ is a connected, compact Euclidean domain for $\nu, \kappa, \sigma^2 > 0$.
- $\mathcal{X} := \mathbb{S}^d$ is the *d-sphere* equipped with the great circle distance, for every $\nu \in (0, 1/2]$ and all $\kappa, \sigma^2 > 0^5$.
- X is a graph with Euclidean edges equipped with the resistance metric for every for every ν ∈ (0, 1/2] and all κ, σ² > 0⁶.

⁶E. Anderes, J. Møller, and J. G. Rasmussen (2020). "Isotropic covariance functions on graphs and their edges". In: Ann. Statist. 48.4, pp. 2478–2503

⁵T. Gneiting (2013). "Strictly and non-strictly positive definite functions on spheres". In: Bernoulli 19.4, pp. 1327–1349

Weakly stationary random fields on \mathbb{R}^d

Setting: $\mathcal{X} \subset \mathbb{R}^d$ and $\varrho|_{\mathcal{X} \times \mathcal{X}}$, $\tilde{\varrho}|_{\mathcal{X} \times \mathcal{X}}$ are restrictions of continuous, positive definite, translation invariant functions $\varrho, \tilde{\varrho} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$.

 $\exists \varrho_0, \widetilde{\varrho}_0 : \mathbb{R}^d \to \mathbb{R} \text{ even} : \quad \varrho(x, x') = \varrho_0(x - x'), \quad \widetilde{\varrho}(x, x') = \widetilde{\varrho}_0(x - x').$

The spectral density f and ρ_0 relate via the inversion formula:

$$\forall \omega \in \mathbb{R}^d : \quad f(\omega) = \frac{1}{(2\pi)^d} (\mathcal{F} \varrho_0)(\omega), \quad (\mathcal{F} \varrho_0)(\omega) \coloneqq \int_{\mathbb{R}^d} e^{-i\omega \cdot x} \varrho_0(x) \, \mathrm{d}x.$$

We define $\mathcal{F}_{\mathcal{X}} \coloneqq \mathcal{F} \circ E^{0}_{\mathcal{X}}$, where $E^{0}_{\mathcal{X}}$ is the zero extension, and $\mathcal{F}_{\mathcal{X}}(L_{2}(\mathcal{X})) = \left\{ \hat{w} : \mathbb{R}^{d} \to \mathbb{C} \mid \exists w \in L_{2}(\mathcal{X}) : \hat{w} = \mathcal{F}_{\mathcal{X}}w \right\} \subset L_{2}(\mathbb{R}^{d};\mathbb{C}).$

The Hilbert space H_f (over \mathbb{R}) is the closure of $\mathcal{F}_{\mathcal{X}}(L_2(\mathcal{X}))$ with respect to norm induced by the inner product

$$(\hat{v}_1, \hat{v}_2)_{H_f} \coloneqq \int_{\mathbb{R}^d} f(\omega) \hat{v}_1(\omega) \overline{\hat{v}_2(\omega)} \, \mathrm{d}\omega, \qquad H_f \coloneqq \overline{\mathcal{F}_{\mathcal{X}}(L_2(\mathcal{X}))}^{\|\cdot\|_{H_f}}.$$



Proposition (Assumptions I and III in terms of spectral densities) Suppose that $C, \widetilde{C} : L_2(\mathcal{X}) \to L_2(\mathcal{X})$ pertain to restrictions (to $\mathcal{X} \times \mathcal{X}$) of translation invariant covariance functions $\varrho, \widetilde{\varrho} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, which have spectral densities $f, \widetilde{f} : \mathbb{R}^d \to [0, \infty)$.

Then, Assumptions I and III are satisfied if and only if:

I' The spaces H_f and $H_{\tilde{f}}$ are isomorphic with equivalent norms, i.e., there exist constants $0 < k \le K < \infty$ such that

$$k\|\hat{v}\|_{H_{f}}^{2} \leq \int_{\mathbb{R}^{d}} \widetilde{f}(\omega)|\hat{v}(\omega)|^{2} d\omega \leq K\|\hat{v}\|_{H_{f}}^{2} \quad \forall \hat{v} \in \mathcal{F}_{\mathcal{X}}(L_{2}(\mathcal{X})).$$

III' There exists $a \in (0, \infty)$ such that the linear operator $\widehat{T}_a := S - a\mathcal{I}_{H_f}$ is compact on H_f , where \mathcal{I}_{H_f} denotes the identity on H_f and $S : H_f \to H_f$ is defined by

$$(S\hat{v}_1,\hat{v}_2)_{H_f}=\int_{\mathbb{R}^d}\widetilde{f}(\omega)\hat{v}_1(\omega)\overline{\hat{v}_2(\omega)}\,\mathrm{d}\omega\qquad\forall\hat{v}_1,\hat{v}_2\in H_f.$$



$$\varrho(x,x') \coloneqq \varrho_0\big(\|x-x'\|_{\mathbb{R}^d}\big), \quad \varrho_0(r) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)} (\kappa r)^{\nu} \mathcal{K}_{\nu}(\kappa r), \quad r \ge 0,$$

Parameters: $\nu, \kappa, \sigma^2 > 0$.

Example (Matérn covariance family)

Assumptions I and III are satisfied if and only if $\nu = \tilde{\nu}$. In this case:

$$\mathbf{a} = \frac{\widetilde{\sigma}^2 \widetilde{\kappa}^{2\nu}}{\sigma^2 \kappa^{2\nu}} \in (0, \infty).$$

For equivalence of the corresponding Gaussian measures, a = 1 is necessary. Indeed, Zhang⁷ and Anderes⁸ showed that, for $\nu = \tilde{\nu}$,

$$\mu \sim \widetilde{\mu} \quad \Longleftrightarrow \quad \begin{cases} \sigma^2 \kappa^{2\nu} = \widetilde{\sigma}^2 \widetilde{\kappa}^{2\nu} & \text{for } d \leq 3, \\ \kappa = \widetilde{\kappa} \text{ and } \sigma^2 = \widetilde{\sigma}^2 & \text{for } d \geq 5. \end{cases}$$

⁸E. Anderes (2010). "On the consistent separation of scale and variance for Gaussian random fields". In: Ann. Statist. 38.2, pp. 870–893

⁷H. Zhang (2004). "Inconsistent estimation and asymptotically equal interpolations in model-based geostatistics". In: *J. Amer. Statist. Assoc.* 99.465, pp. 250–261

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d

Common eigenbasis

Generalized Whittle–Matérn fields Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Covariance operators with the same eigenbasis

Corollary

Suppose that C, \widetilde{C} are self-adjoint, positive definite, trace-class operators on $L_2(\mathcal{X}, \nu_{\mathcal{X}})$ which diagonalize with respect to the same orthonormal basis $\{e_j\}_{j \in \mathbb{N}}$ for $L_2(\mathcal{X}, \nu_{\mathcal{X}})$, i.e., there are $\{\gamma_j\}_{j \in \mathbb{N}}, \{\widetilde{\gamma}_j\}_{j \in \mathbb{N}} \subset (0, \infty)$ s.t.

 $Ce_j = \gamma_j e_j$ and $\widetilde{C}e_j = \widetilde{\gamma}_j e_j$ $\forall j \in \mathbb{N}$.

Consider $\mu := \mathsf{N}(0, \mathcal{C})$ and $\widetilde{\mu} := \mathsf{N}(0, \widetilde{\mathcal{C}})$.

- The Cameron–Martin spaces for μ and μ̃ are isomorphic if and only if there exist c₋, c₊ ∈ ℝ₊ such that γ̃_j/γ_j ∈ [c₋, c₊] for all j ∈ ℕ.
- μ and $\widetilde{\mu}$ are equivalent if and only if $\sum_{j \in \mathbb{N}} (\widetilde{\gamma}_j / \gamma_j 1)^2 < \infty$.
- Assumptions I and III are satisfied if and only if there exists a constant a ∈ (0,∞) such that lim_{i→∞} γ_i/γ_i = a.



Consider the shifted negative Dirichlet Laplacian:

 $Lv \coloneqq \left(-\Delta + \kappa^2\right) v, \qquad v \in \mathcal{D}(L) \coloneqq H^2(\mathcal{D}) \cap H^1_0(\mathcal{D}),$

where $\mathcal{D} \not\subseteq \mathbb{R}^d$ is a bounded open Lipschitz domain.

Corollary ("Classical" Whittle-Matérn fields)

Let $d \in \mathbb{N}$, $\beta, \widetilde{\beta} > d/_4$, $\tau, \widetilde{\tau} > 0$, and let L, \widetilde{L} have shift parameters $\kappa^2 \ge 0$ and $\widetilde{\kappa}^2 \ge 0$, respectively. Consider on $L_2(\mathcal{D})$ the Gaussian measures

$$\mu = \mathsf{N}\big(0, \tau^{-2} L^{-2\beta}\big) \quad \text{and} \quad \widetilde{\mu} = \mathsf{N}\big(0, \widetilde{\tau}^{-2} \widetilde{L}^{-2\beta}\big).$$

- The Cameron–Martin spaces for μ and $\tilde{\mu}$ are isomorphic, with equivalent norms, if and only if $\beta = \tilde{\beta}$.
- μ and $\widetilde{\mu}$ are equivalent if and only if

$$\begin{cases} \beta = \widetilde{\beta} \text{ and } \tau = \widetilde{\tau} & \text{if } d \leq 3, \\ \beta = \widetilde{\beta}, \ \tau = \widetilde{\tau} \text{ and } \kappa^2 = \widetilde{\kappa}^2 & \text{if } d \geq 4. \end{cases}$$

• For any $d \in \mathbb{N}$, Assumptions I & III are fulfilled if and only if $\beta = \widetilde{\beta}$.

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis

Generalized Whittle-Matérn fields

Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Generalized Whittle–Matérn fields on $\mathcal{D} \subsetneq \mathbb{R}^d$

Next, we consider Gaussian measures on $L_2(\mathcal{D})$, $\mathcal{D} \subseteq \mathbb{R}^d$, of the form

$$\mu_d(m;\beta,\mathbf{a},\kappa) \coloneqq \mathsf{N}(m,L^{-2\beta}),$$

where $m \in L_2(\mathcal{D})$, $\beta > d/4$ and

$$Lv = -\nabla \cdot (\mathbf{a} \nabla v) + \kappa^2 v, \qquad v \in \mathscr{D}(L) \subseteq L_2(\mathcal{D}) \cap H_0^1(\mathcal{D}).$$

We suppose that a and κ and the domain $\mathcal{D} \subset \mathbb{R}^d$ satisfy the following.

Setting WM

i. $\mathbf{a}: \overline{\mathcal{D}} \to \mathbb{R}^{d \times d}$ is symmetric and uniformly positive definite, i.e.,

 $\exists a_0 > 0: \quad \forall \xi \in \mathbb{R}^d: \quad \operatorname{ess\,inf}_{s \in \mathcal{D}} \xi^\top \boldsymbol{a}(s) \xi \geq a_0 \|\xi\|_{\mathbb{R}^d}^2,$

and $\mathbf{a} = (\mathbf{a}_{jk})_{j,k=1}^d$ is smooth, $\mathbf{a}_{jk} \in C^{\infty}(\overline{\mathcal{D}})$ for all $j, k \in \{1, \dots, d\}$. ii. $\kappa : \overline{\mathcal{D}} \to \mathbb{R}$ is smooth, $\kappa \in C^{\infty}(\overline{\mathcal{D}})$.

iii. The domain $\mathcal{D} \subset \mathbb{R}^d$ has a smooth boundary $\partial \mathcal{D}$ of class C^{∞} .

TUDelft

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis

Generalized Whittle–Matérn fields Isomorphic Cameron–Martin spaces

Equivalence of measures and asymptotically optimal linear predict Summary and simulations Lemma (Cameron–Martin space for $\mu_d(m; \beta, a, \kappa)$)

Suppose Setting WM. For every $\beta > d/4$, the Cameron–Martin space of the Gaussian measure $\mu_d(m; \beta, a, \kappa)$ is

$$\mathcal{C}^{1/2}(L_2(\mathcal{D})) = \dot{H}_L^{2\beta} \coloneqq \mathscr{D}(L^\beta) \subseteq L_2(\mathcal{D}), \qquad \|\mathbf{v}\|_{2\beta,L} \coloneqq \|L^\beta \mathbf{v}\|_{L_2(\mathcal{D})}.$$

It is a subspace of the Sobolev space $\mathsf{H}^{2eta}(\mathcal{D})$ and

$$\left(\dot{H}_{L}^{2\beta}, \|\cdot\|_{2\beta, L}\right) \hookrightarrow \left(H^{2\beta}(\mathcal{D}), \|\cdot\|_{H^{2\beta}(\mathcal{D})}\right) \hookrightarrow \left(C^{0}(\overline{\mathcal{D}}), \|\cdot\|_{C^{0}(\overline{\mathcal{D}})}\right)$$

Furthermore, provided that $2\beta \notin \mathcal{E}$, where

$$\mathscr{E} \coloneqq \{2k + \frac{1}{2} \colon k \in \mathbb{N}_0\},\$$

we have the identification

$$\dot{H}_{L}^{2\beta} = \left\{ v \in H^{2\beta}(\mathcal{D}) : \left(\kappa^{2} - \nabla \cdot (\mathbf{a} \nabla) \right)^{j} v = 0 \text{ in } L_{2}(\partial \mathcal{D}) \quad \forall j = 0, \dots, \lfloor \beta - \frac{1}{4} \rfloor \right\},$$

and on $\dot{H}_{L}^{2\beta}$ the Sobolev norm $\|\cdot\|_{H^{2\beta}(\mathcal{D})}$ and $\|\cdot\|_{2\beta,L}$ are equivalent.

Theorem (Isomorphic Cameron–Martin spaces)

Suppose Setting WM for each of the parameter tuples (\mathbf{a}, κ) , $(\widetilde{\mathbf{a}}, \widetilde{\kappa})$ and for $\mathcal{D} \subseteq \mathbb{R}^d$. Let $\beta, \widetilde{\beta} > d/4$ be such that $2\beta \notin \mathscr{E}$.

The Cameron-Martin spaces of two Gaussian measures

 $\mu_d(0; \beta, \boldsymbol{a}, \kappa)$ and $\mu_d(0; \widetilde{\beta}, \widetilde{\boldsymbol{a}}, \widetilde{\kappa})$

are isomorphic with equivalent norms if and only if $\beta = \tilde{\beta}$ and for every $j \in \mathbb{N}_0$ with $j \leq \lfloor \beta - 5/4 \rfloor$ the following hold:

$$\forall v \in \dot{H}_{L}^{2\beta} : (\kappa^{2} - \nabla \cdot (\boldsymbol{a}\nabla))^{j} (\delta_{\kappa^{2}} - \nabla \cdot (\delta_{\boldsymbol{a}}\nabla)) v = 0 \text{ in } L_{2}(\partial \mathcal{D}),$$

$$\forall \widetilde{v} \in \dot{H}_{\widetilde{I}}^{2\beta} : (\widetilde{\kappa}^{2} - \nabla \cdot (\widetilde{\boldsymbol{a}}\nabla))^{j} (\delta_{\kappa^{2}} - \nabla \cdot (\delta_{\boldsymbol{a}}\nabla)) \widetilde{v} = 0 \text{ in } L_{2}(\partial \mathcal{D}).$$
(BCs)

Here, $\delta_{\kappa^2}(s) \coloneqq \widetilde{\kappa}^2(s) - \kappa^2(s)$ and $\delta_a(s) \coloneqq \widetilde{a}(s) - a(s)$ for all $s \in \overline{\mathcal{D}}$.

 \Rightarrow The behavior of δ_{κ^2} and δ_a on the boundary $\partial \mathcal{D}$ matters!

ŤUDelft

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis

Generalized Whittle-Matérn fields

Isomorphic Cameron-Martin spaces

Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Conditions on the parameters for equivalent measures

Theorem (Characterizing equivalence of the measures μ and $\tilde{\mu}$)

Suppose Setting WM for each of the parameter tuples (a, κ) , $(\widetilde{a}, \widetilde{\kappa})$ and for $\mathcal{D} \not\subseteq \mathbb{R}^d$. Let $m, \widetilde{m} \in L_2(\mathcal{D})$ and $\beta, \widetilde{\beta} > d/4$ be such that $2\beta \notin \mathscr{E}$.

- In dimension $d \leq 3$, the Gaussian measures $\mu_d(m; \beta, a, \kappa)$ and $\mu_d(\widetilde{m}; \widetilde{\beta}, \widetilde{a}, \widetilde{\kappa})$ are equivalent if and only if
 - $\beta = \widetilde{\beta}$,
 - the boundary conditions (BCs) hold for every $j = 0, 1, ..., \lfloor \beta 5/4 \rfloor$,

•
$$m - \widetilde{m} \in \dot{H}_L^{2\beta}$$
,

- *a* = ã.
- In dimension $d \ge 4$, the Gaussian measures $\mu_d(m; \beta, a, \kappa)$ and $\mu_d(\widetilde{m}; \widetilde{\beta}, \widetilde{a}, \widetilde{\kappa})$ are equivalent if and only if

•
$$\beta = \widetilde{\beta}$$
,
• $\kappa^2 = \widetilde{\kappa}^2$,
• $m - \widetilde{m} \in \dot{H}_{L}^{2\beta}$,

ŤUDelft

Conditions on the parameters for optimal linear prediction

Theorem (Uniformly asymptotically optimal linear prediction)

Suppose Setting WM for each of the parameter tuples (\mathbf{a}, κ) , $(\widetilde{\mathbf{a}}, \widetilde{\kappa})$ and for $\mathcal{D} \not\subseteq \mathbb{R}^d$. Let $m, \widetilde{m} \in L_2(\mathcal{D})$ and $\beta, \widetilde{\beta} > d/4$ be such that $2\beta \notin \mathscr{E}$. Consider the Gaussian measures

 $\mu_d(m; \beta, \boldsymbol{a}, \kappa)$ and $\mu_d(\widetilde{m}; \widetilde{\beta}, \widetilde{\boldsymbol{a}}, \widetilde{\kappa})$

Then, the Assumptions I–III (for uniformly asymptotically optimal linear prediction) are satisfied if and only if

- $\beta = \widetilde{\beta}$,
- the boundary conditions (BCs) hold for every $j = 0, 1, ..., \lfloor \beta 5/4 \rfloor$,
- $m \widetilde{m} \in \dot{H}_L^{2\beta}$,
- here exists a constant c > 0 such that $ca = \tilde{a}$.

1 Necessary and sufficient conditions for asymptotic optimality

Linear prediction on compact metric spaces The assumptions and main result

2 Applications

Weakly stationary random fields on \mathbb{R}^d Common eigenbasis

Generalized Whittle-Matérn fields

Isomorphic Cameron–Martin spaces Equivalence of measures and asymptotically optimal linear prediction Summary and simulations

Summary

Let $\mu := \mu_d(0; \beta, \mathbf{a}, \kappa)$, $\widetilde{\mu} := \mu_d(0; \widetilde{\beta}, \widetilde{\mathbf{a}}, \widetilde{\kappa})$ be Gaussian measures for generalized Whittle–Matérn fields with parameters $(\beta, \mathbf{a}, \kappa)$ resp. $(\widetilde{\beta}, \widetilde{\mathbf{a}}, \widetilde{\kappa})$.

	Interval for β , assuming that $\beta \notin \{k + 1/4 : k \in \mathbb{N}\}$		
Conditions for	(d/4, 9/4)	(9/4,13/4)	$(13/4,\infty)$
Asymptotically optimal linear prediction	$\beta = \widetilde{\beta}, \ c\mathbf{a} = \widetilde{\mathbf{a}}$ for some $c \in (0, \infty)$	$ \begin{vmatrix} \beta = \widetilde{\beta}, \ \mathbf{ca} = \widetilde{\mathbf{a}}, \\ \left(\mathbf{a}\nabla\delta_{c,\kappa^2}\right)\Big _{\partial\mathcal{D}} \cdot \mathbf{n} = 0 $	$\beta = \widetilde{\beta}, \ ca = \widetilde{a} \\ + \text{ b.c. on } \delta_{c,\kappa^2}$
Equivalence of measures in dimension $d \le 3$	$\beta = \widetilde{\beta}, \ \mathbf{a} = \widetilde{\mathbf{a}}$	$\begin{vmatrix} \boldsymbol{\beta} = \widetilde{\boldsymbol{\beta}}, \ \mathbf{a} = \widetilde{\mathbf{a}}, \\ \left(\mathbf{a} \nabla \delta_{1,\kappa^2}\right) \Big _{\partial \mathcal{D}} \cdot \mathbf{n} = 0 \end{aligned}$	$\beta = \widetilde{\beta}, \ \mathbf{a} = \widetilde{\mathbf{a}}$ + b.c. on δ_{1,κ^2}
Equivalence of measures in dimension $d \ge 4$	β =	$\widetilde{eta}, \mathbf{a} = \widetilde{\mathbf{a}}, \kappa^2 = \widetilde{\kappa}^2$	

 $\delta_{c,\kappa^2}(s) \coloneqq \widetilde{\kappa}^2(s) - c\kappa^2(s)$, and **n** is the outward pointing normal on $\partial \mathcal{D}$.

Simulation 1: The difference between κ^2 and **a**

$$(-\nabla \cdot (\boldsymbol{a} \nabla) + \kappa^2)^{\beta}(\tau Z) = \mathcal{W} \text{ in } \mathcal{D} = (0,1).$$

True model: $\beta = 1$, $a \equiv 1$, $\kappa^2 \equiv 1200$, and $\tau = \frac{1}{2}\kappa^{-3/2}$.

Two misspecified models: correct values of β, τ , and we set

$$\left(\kappa^{2}(s), \boldsymbol{a}(s)\right) = \begin{cases} \left(1200f(s)^{-1}, 1\right) & \text{for model } 1, \\ \left(1200, f(s)\right) & \text{for model } 2, \end{cases} \quad s \in \overline{\mathcal{D}} = [0, 1],$$

where $f(s) \coloneqq 1 + \frac{1}{2} \operatorname{erf}\left(\frac{\delta(s-0.5)}{\sqrt{2}}\right)$.

As a measure of accuracy, we use

$$\mathcal{E}_n(h) \coloneqq \frac{\mathsf{E}\big[(\widetilde{h}_n - h)^2\big]}{\mathsf{E}\big[(h_n - h)^2\big]} - 1.$$

We predict $Z(x_0)$ as well as the integrals $I_{\ell} := (Z, e_{\ell})_{L_2(\mathcal{D})}$ and set $\mathcal{E}_{l,n}^{\max} := \max \{ \mathcal{E}_{l,n}^{\ell} : n+1 \le \ell \le N \}, \qquad \mathcal{E}_{l,n}^{\ell} := \mathcal{E}_n(I_{\ell}), \quad \ell \in \{n+1, \dots, N\}.$

Results of Simulation 1



Figure: The results for model 1 (black) and model 2 (red) for the first example with integral observations (left) and point observations (right).

Solid lines correspond to $\delta = 1$, dashed to $\delta = 10$, and dotted to $\delta = 100$.



Simulation 2: The effect of the smoothness parameter β For $\beta \in \{1, 2, 3\}$, we consider

$$(-\nabla \cdot (\boldsymbol{a} \nabla) + \kappa^2)^{\beta} (\tau Z) = \mathcal{W} \text{ in } \mathcal{D} = (0, 1).$$

True model: $\boldsymbol{a} \equiv 1$, $\kappa^2 \equiv 100(4\beta - 1)$, and $\tau > 0$.

Two misspecified models: correct values of β , \boldsymbol{a} , τ , and we set

$$\kappa^{2}(s) = 100(4\beta - 1) \cdot \begin{cases} 1 - 1.5s^{2} + s^{3} & \text{for model } 1, \\ 1 + s - 1.5s^{3} & \text{for model } 2, \end{cases} \quad s \in \overline{\mathcal{D}} = [0, 1].$$

We again predict the integrals $I_{\ell} := (Z, e_{\ell})_{L_2(\mathcal{D})}$ and consider

$$\mathcal{E}_{I,n}^{\max} \coloneqq \max \{ \mathcal{E}_{I,n}^{\ell} : n+1 \le \ell \le N \}, \qquad \mathcal{E}_{I,n}^{\ell} \coloneqq \mathcal{E}_n(I_{\ell}), \quad \ell \in \{n+1,\ldots,N\},$$

where

$$\mathcal{E}_n(h) \coloneqq \frac{\mathsf{E}\big[(\widetilde{h}_n - h)^2\big]}{\mathsf{E}\big[(h_n - h)^2\big]} - 1.$$



Results of Simulation 2



Left: The results for model 1 (black) and model 2 (red) in the second example, with $\beta = 1$ (solid), $\beta = 2$ (dashed), and $\beta = 3$ (dotted).

Right: κ^2 for the two models when $\beta = 1$.

References

- K. Kirchner and D. Bolin (2020). Necessary and sufficient conditions for asymptotically optimal linear prediction of random fields on compact metric spaces. To appear in: Annals of Statistics. Preprint: arXiv:2005.08904.
- D. Bolin and K. Kirchner (2021). Equivalence of measures and asymptotically optimal linear prediction for Gaussian random fields with fractional-order covariance operators. Preprint: arXiv:2101.07860.

Thank you for your attention!