ARGUMENTWISE INVARIANT KERNELS FOR THE APPROXIMATION OF INVARIANT FUNCTIONS

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Abstract. Modeling a deterministic function using gaussian processes and Kriging relies on the selection of an adapted covariance kernel. Similarly, the use of approximation methods from the theory of reproducing kernel Hilbert spaces bases on the choice of a positive definite kernel. When some prior information is available concerning symmetries or arbitrary algebraic invariances of the function to be approximated, it is clearly unreasonable not trying to use it at the stage of kernel selection. We propose a characterization of kernels which associated square-integrable processes have their paths invariant under the action of a finite group. We then give examples of such pathwise invariant processes, built on the basis of stationary and unstationary gaussian processes. The approximation of a function from the structural reliability literature, invariant under the action of a group of order 4, finally allows comparing several Kriging approaches, with different symmetrized kernels. The obtained results confirm the practical interest of the proposed method, at the same time in terms of improved prediction and of conditional simulations respecting prescribed invariances.

Résumé La modélisation d'une fonction déterministe par un processus gaussien nécessite de sélectionner un noyau de covariance. De même, l'utilisation de méthodes d'approximation de la théorie des espaces de Hilbert à noyau reproduisant repose sur le choix d'un noyau défini positif. Lorsque l'on dispose a priori d'informations sur les symétries de la fonction que l'on souhaite approximer, il est fort dommageable de ne pas les utiliser à l'étape du choix du noyau. Nous proposons une caractérisation des noyaux de covariance dont les processus associés possèdent des réalisations invariantes par l'action d'un groupe fini. Nous donnons ensuite des exemples de tels processus, et discutons des propriétés du Krigeage lorsque de tels noyaux sont utilisés. L'approximation d'une fonction issue de la litérature en fiabilité des structures, invariante sous l'action d'un groupe d'ordre 4, permet finalement de comparer plusieurs approches incluant des symmétrisation de noyaux ou de plans. Les résultats obtenus confirment l'intŕt pratique de la méthode proposée, aussi bien en termes de prediction que de simulations conditionnelles.

Contents

1. Introduction

Positive definite[1] (p.d.) kernels play a central role in several contemporary functional approximation methods, ranging from regularization techniques within the theory of *Reproducing Kernel Hilbert Spaces* (RKHS) to *Gaussian Process Regression* (GPR) in machine learning. One of the reason for that is presumably the following particularly elegant predictor, common solution to approximation in both framworks. Indeed, if scalar responses $\mathbf{y} := (y_1, \ldots, y_n) \in \mathbb{R}$ $(n \in \mathbb{N} - \{0\})$ are observed for n instances $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$ of a d-dimensional input variable (D is here assumed to be a compact subset of $\mathbb{R}^d$, $d \in \mathbb{N} - \{0\}$), the function

$$m : \mathbf{x} \in D \longrightarrow m(\mathbf{x}) = \mathbf{k}(\mathbf{x})' K^{-1} \mathbf{y}, \tag{1}$$

is at the same time the best approximation of any function f in the RKHS of kernel k subject to $f(\mathbf{x}_i) = y_i$ $(1 \leq i \leq n)$, and the GPR ("Simple Kriging") predictor of any squared-integrable centered random field $(Y_{\mathbf{x} \in D})_{\mathbf{x} \in D}$ of covariance kernel k subject to $Y_{\mathbf{x}_i} = y_i$ $(1 \leq i \leq n)$. $k : D \times D \longrightarrow \mathbb{R}$ stands here for an aribitrary p.d. kernel, with $\mathbf{k}(\mathbf{x}) := (k(\mathbf{x}, \mathbf{x}_1), \ldots, k(\mathbf{x}, \mathbf{x}_n))$ and $K := (k(\mathbf{x}_i, \mathbf{x}_j))_{1, i \leq j \leq n}$ (assumed invertible here and in the sequel).

In practical situations (e.g., when the y_i's steem from the output of an expensive-to-evaluate deterministic numerical simulator, say $y : D \to \mathbb{R}$), the choice of k is generally far from being trivial. Unless there is a strong prior in favour of a specific kernel of parametric family of kernel, the usual *modus operandi* to choose k in GPR (when d is too high and/or n too low for a geostatistical variogram estimation) is to rely on well-known families of kernels, and to perform a classical (Maximum Likelihood, Cross-Validation)

1. We use here the term p.d. for what some authors also call "non-negative definite".

or bayesian inference of the underlying parameters based on data. For example, most GPR of Kriging softwares offer different options for the underlying kernel, often restricted to stationary but anisotropic correlations like the Matérn or generalized exponential kernels, allowing the user to choose between different levels of regularity. This is in fact based on solid mathematical results concerning the link between the regularity of covariance kernels and the mean square properties of squared integrable random fields (or even a.s. properties in the case of Gaussian Random Fields [2]).

A weak point of such an approach, however, is that not all phenomena can reasonably be approximated by stationary random fields, even with a well-chosen level of regularity and a successful estimation of the kernel parameters. In order to circumvent that limitation, several non-stationary approaches have been proposed in the recent literature, including convolution kernels (see [28] or [23]), kernels incorporating non-linear transformations of the input space ([19, 4, 43]), or treed gaussian processes ([18]), to cite an excerpt of some of the most popular approaches.

Our intent here is to address a specific question related to the choice of k: assuming a known geometric or algebraic invariance of the phenomenon under study, is it possible to incorporate it directly in a kernel-based approximation method like GPR or RKHS regularization? More precisely, given a function y invariant under a measurable action Φ of some finite group G on D, is it possible to construct a metamodel respecting that invariance?

Here we investigate classes of kernels leading to metamodels m inheriting the invariances of y. In the particular case of a GPR interpretation, the proposed kernels enable a deeper embedding of the prescribed invariance in the metamodel since the obtained random fields have invariant paths (up to a modification). Note that the proposed approach is rather complementary to the non-stationary kernels evocated above than in concurrence with them. Our main goals are indeed to understand to what extent kernel methods are compatible with invariance assumptions, what kind of kernels are suitable to model invariant functions, and how to construct such kernels based on existing (stationary or already non-stationary) kernels.

The paper is organized as follows. In section 2, we recall some fundamental algebraic definitions (2.1) and random fields technical notions useful in the sequel (2.2), followed by an overview with discussion on the existing work concerning invariant kernels and random fields. The main results are give in section 3. A characterization of positive definite kernels leading to invariant random fields is given (3.1), and several properties of the corresponding metamodels are discussed (3.2). 3.3 is dedicated to the RKHS interpretation of such kernels. Application results are then presented in section 4, first with illustrations on toy examples (4.1), and then with a test case from the reliability literature. Finally, a few concluding remarks and a discussion on perspectives and forthcoming research questions are given in section 5.

2. Definitions and classical results

2.1. **Group actions and invariant functions.** Let $(G,*)$ be a group and D a set. We denote by e the neutral element of G.

Definition 1. *A (left) action of the group G on D is a map $\Phi : (g,x) \in D \times E \longrightarrow g.x := \Phi(g,x) \in D$ such that*
- $x \in D \longmapsto \Phi(e,x)$ *is the identitity of D, i.e. $\forall x \in D,\ \Phi(e,x) = x$,*
- $\forall x \in D,\ \forall g, g' \in G,\ \Phi(gg', x) = \Phi(g, \Phi(g', x))$.

Definition 2. *The orbit of a points $\mathbf{x} \in D$ under the action Φ is the set*

$$\mathcal{O}(x) := \{g.x,\ g \in G\}, \tag{2}$$

constituted of images of x by the action of G. $\mathbf{x}$ is a fixed point of the action when $\forall g \in G,\ g.x = x$. The fixator of $A \subset D$ in G is defined by $Fix_{\Phi}(x) := \{g \in G \mid \forall a \in A,\ g.a = a\}$, and the stabilizer of A by $Stab_{\Phi}(A) := \{g \in G \mid \forall a \in A,\ g.a \in A\}$.

Definition 3. *Le F be an arbitrary set. A map $y : D \longrightarrow F$ is said invariant by Φ, or invariant under the action of the group G, when*

$$\forall \mathbf{x} \in D,\ \forall g \in G,\ y(g.\mathbf{x}) = y(\mathbf{x}) \tag{3}$$

It amounts to requiring that y is constant on the orbits of Φ.

2.2. **Random Fields.** We borrow here a few definitions from the book [31], with a few minor changes in the notations.

Definition 4. *Two random fields Y and Y' defined respectively on the probability spaces $(\Omega, \mathcal{F}, \mathbb{P})$ and $(\Omega', \mathcal{F}', \mathbb{P}')$, and sharing a common state space $(D, \mathcal{D})$, are said equivalent if for any finite sequences of points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$ and events $A_1, \ldots, A_n \in \mathcal{D}$,*

$$\mathbb{P}\left(Y_{\mathbf{x}_1} \in A_1, \ldots, Y_{\mathbf{x}_n} \in A_n\right) = \mathbb{P}'\left(Y'_{\mathbf{x}_1} \in A_1, \ldots, Y'_{\mathbf{x}_n} \in A_n\right) \tag{4}$$

One also says in that case that each one of these random fields is a version of the other, or that both are versions of the same random field. In other words, two random fields are versions of each other whenever they have the same finite-dimensional distributions.

Definition 5. *Two random fields Y et Y' defined on the same probability space $(\Omega, \mathcal{F}, \mathbb{P})$ are said to be modifications of each other when for all $\mathbf{x} \in D$,*

$$Y_{\mathbf{x}} = Y'_{\mathbf{x}} \quad \mathbb{P}\text{-}p.s. \tag{5}$$

They are said indistinguishable when for $\mathbb{P}$-almost all $\omega \in \Omega$,

$$\forall \mathbf{x} \in D,\ Y_{\mathbf{x}}(\omega) = Y'_{\mathbf{x}}(\omega) \tag{6}$$

As prcised in ([31], p. 18), if Y and Y' are modifications of each other, they clearly are versions of the same random field. A slightly less straightforward result is that if two random fields modifications of each other are almost surely continuous, then they are indistinguishable

Definition 6. *Y is said to have all its paths invariant under the action of G whenever*

$$\forall \omega \in \Omega,\ \forall \mathbf{x} \in D,\ \forall g \in G,\ Y_{\mathbf{x}}(\omega) = Y_{g.\mathbf{x}}(\omega) \tag{7}$$

2.3. **Classical results about invariant kernels and random fields.**

2.3.1. *Stationarity, isotropy: invariance-related notions in geostatistics.* A very classical notion in spatial statistics, and more generally in the literature of random processes (including time series in the first place), is the one of *second order* or *weak stationarity*. A centered squared-integrable random field Y is said weakly stationary whenever $cov(Y_{\mathbf{x}}, Y_{\mathbf{x}'})$ is a function of $\mathbf{x}-\mathbf{x}'$ (here $\mathbf{x}, \mathbf{x}' \in D$) or equivalently that for any $\mathbf{x} \in D$ and $\mathbf{h}$ such that $\mathbf{x}+\mathbf{h} \in D$, $cov(Y_{\mathbf{x}+\mathbf{h}}, Y_{\mathbf{x}})$ is depending only on $\mathbf{h}$ and not on $\mathbf{x}$. In other words, the covariance kernel of Y is such that for any pair of points $\mathbf{x}, \mathbf{x}' \in D$ and translation $T_{\mathbf{h}} : \mathbf{x} \in D \longrightarrow T_{\mathbf{h}}(\mathbf{x}) := \mathbf{x}+\mathbf{h}$ with $\mathbf{x}+\mathbf{h}, \mathbf{x}'+\mathbf{h} \in D$,

$$k(T_{\mathbf{h}}(\mathbf{x}), T_{\mathbf{h}}(\mathbf{x}')) = k(\mathbf{x}, \mathbf{x}') \tag{8}$$

Likewise, a centered random field Y defined over some subset D of a euclidean space is said to be *weakly isotropic* whenever $cov(Y_{\mathbf{x}}, Y_{\mathbf{x}'})$ depends only on the norm-induced distance between $\mathbf{x}$ and $\mathbf{x}'$, i.e. $k(\mathbf{x}, \mathbf{x}')$ is a function of $||\mathbf{x}-\mathbf{x}'||$. Again, this may be written as an invariance of the kernel under the simultaneous transformation of both arguments:

$$k(R(\mathbf{x}), R(\mathbf{x}')) = k(\mathbf{x}, \mathbf{x}') \tag{9}$$

where R belongs this time to the more general class of isometries. Both latter invariances are in fact particular cases of the following definition given by Parthasarathy and Schmidt in [29]:

Definition 7. *k is said invariant under the action of G on D when*

$$\forall g \in G, \forall \mathbf{x}, \mathbf{x}' \in D,\ k(g.\mathbf{x}, g.\mathbf{x}') = k(\mathbf{x}, \mathbf{x}') \tag{10}$$

3. Main results

3.1. **A characterization of kernels leading to invariant fields.**

Before stating the main result of the paper, we need to introduce a new notion, generalizing the notion of invariant kernel presented in the last section.

Definition 8. *A kernel k is said argumentwise invariant under the action of G on D when*

$$\forall g, g' \in G, \forall \mathbf{x}, \mathbf{x}' \in D,\ k(g.\mathbf{x}, g'.\mathbf{x}') = k(\mathbf{x}, \mathbf{x}') \tag{11}$$

One can notice that eq.(10) corresponds to the particular case of eq.(11) where $g = g'$. As we will see now, this second kind of kernels corresponds to much stronger invariance properties of the associated random fields.

Theorem 3.1. *(kernels characterizing invariant fields) Let G be a finite group of order $r \in \mathbb{N} - \{0\}$ acting on D via the action Φ, and $(Y_{\mathbf{x}})_{\mathbf{x}\in D}$ a centered squared-integrable random field over D. Y has all its paths invariant* *under Φ (up to a modification) if and only if its covariance kernel k is argumentwise invariant under Φ.*

Proof. Let us first assume that Y has all its paths invariant under Φ up to a modification. Then, there exist a process $\widetilde{Y}$ having all its paths invariant under Φ and such that $\forall \mathbf{x} \in D,\ \mathbb{P}(Y_{\mathbf{x}} = \widetilde{Y}_{\mathbf{x}}) = 1$. It is then clear that the covariance kernels of both fields, say k_Y and $k_{\widetilde{Y}}$, coincide. Now, by invariance of $\widetilde{Y}$'s paths, we have that $\forall \mathbf{x} \in D\ \forall g \in G\ \forall \omega \in \Omega,\ \widetilde{Y}_{\mathbf{x}}(\omega) = \widetilde{Y}_{g.\mathbf{x}}(\omega)$, so that in particular $\forall \mathbf{x} \in D\ \forall g, g' \in G$:

$$k_{\widetilde{Y}}(g.\mathbf{x}, g'.\mathbf{x}') = cov[\widetilde{Y}_{g.\mathbf{x}}, \widetilde{Y}_{g'.\mathbf{x}'}] = cov[\widetilde{Y}_{\mathbf{x}}, \widetilde{Y}_{g'.\mathbf{x}'}] = cov[\widetilde{Y}_{\mathbf{x}}, \widetilde{Y}_{\mathbf{x}'}] = k_{\widetilde{Y}}(\mathbf{x}, \mathbf{x}')$$

Reciprocally, let us assume now that k_Y is argumentwise invariant under Φ. Let us denote by $A \subset D$ a fundamental domain for ϕ, and by $\pi_A : D \longrightarrow A$ the projector mapping any $\mathbf{x} \in D$ to its representer $\pi_A(\mathbf{x}) \in A$, i.e. to the point of A being in the same orbit. We then define the random field $\widetilde{Y}$ by

$$\forall \mathbf{x} \in D\ \widetilde{Y}_{\mathbf{x}} := Y_{\pi_A(\mathbf{x})}$$

By construction, $\widetilde{Y}$ has all its paths invariant under Φ. Now, for any $\mathbf{x} \in D$, there exists $g \in G$ such that $\pi_A(\mathbf{x}) = g.\mathbf{x}$. Subsequently,

$$\begin{aligned} var[Y_{\mathbf{x}} - \widetilde{Y}_{\mathbf{x}}] &= var[Y_{\mathbf{x}} - Y_{g.\mathbf{x}}] \\ &= k(\mathbf{x}, \mathbf{x}) + k(g.\mathbf{x}, g.\mathbf{x}) - 2k(\mathbf{x}, g.\mathbf{x}) = 0, \end{aligned}$$

so that $\mathbb{P}(Y_{\mathbf{x}} = \widetilde{Y}_{\mathbf{x}}) = 1$, and Y is a modification of a random field having all its paths invariant under Φ. □

Remark 1. *A fundamental domain A is such that every orbit has a unique representer in A, and $\bigcup_{g \in G} g.A = D$. However, the $g.A$'s ($g \in G$) are not necessarily disjoints. For example, if $G = \mathbb{Z}/2\mathbb{Z}$, $D = \mathbb{R}$, and $\Phi : (g, x) \in (\mathbb{Z}/2\mathbb{Z}) \times \mathbb{R} \longrightarrow \mathbb{R}$ is the action defined by $\Phi(\bar{1}, x) = -x$, $A = [0, +\infty[$ is a fundamental domain containing 0, but $0 \in \bar{1}.A =]-\infty, 0]$ too. Consequently, when decomposing an invariant process over the orbits of A, one must account for the points appearing in several $g.A$'s by divinding by the number of appearances, characterized by the cardinal of their stabilizers:*

$$\forall \mathbf{x} \in D,\ Y_{\mathbf{x}} = \sum_{g \in G} Y_{\mathbf{x}} \frac{\mathbf{1}_{g.A}(\mathbf{x})}{\# Stab_{\Phi}(\mathbf{x})} = \sum_{g \in G} Z_{g.\mathbf{x}} \tag{12}$$

where $Z_{\mathbf{x}} := Y_{\mathbf{x}} \frac{\mathbf{1}_A(\mathbf{x})}{\# Stab_{\Phi}(\mathbf{x})}$. Denoting Z's kernel by k_Z, we get in particular

$$\forall \mathbf{x}, \mathbf{x}' \in D\ k_Y(\mathbf{x}, \mathbf{x}') = Cov\left[\sum_{g \in G}^{m} Z_{g.\mathbf{x}}, \sum_{g' \in G}^{m} Z_{g'.\mathbf{x}'}\right] = \sum_{(g,g') \in G^2} k_Z(g.\mathbf{x}, g'.\mathbf{x}'),$$

whereof the argumentwise invariance of k_Y clearly appears.

Example 1. *Let Y be a centered gaussian process indexed by $\mathbb{R}$, with covariance kernel $k_Y : x, x' \in \mathbb{R} \longrightarrow k_X(x, x') = e^{-|x-x'|} \in \mathbb{R}$ (often called the Ornstein-Uhlenbeck process, Cf. [31] sec. 1.3), and $\Phi : (g, x) \in (\mathbb{Z}/2\mathbb{Z}) \times \mathbb{R} \longrightarrow \mathbb{R}$ the action of $G = \mathbb{Z}/2\mathbb{Z}$ on $\mathbb{R}$ previously considered. The process S obtained by symmetrization of Y's restriction to $A := [0, +\infty[$, defined by $S_x = \frac{1}{1+\mathbf{1}_{\{0\}}(x)} Y_x \mathbf{1}_{[0,+\infty[}(x) + \frac{1}{1+\mathbf{1}_{\{0\}}(x)} Y_x \mathbf{1}_{[0,+\infty[}(-x)$, has all its paths invariant under Φ. Its covariance kernel is given by $\forall x, x' \in \mathbb{R},\ k_S(x, x') = e^{-||x|-|x'||}$. Let us notice that S, symmetrized of the stationary process Y, is obviously not second order stationary.*

Example 2. *Let Y be a centered gaussian process indexed by $\mathbb{R}^2$, with covariance kernel $k_Y : \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2 \longrightarrow e^{-||\mathbf{x}-\mathbf{x}'||^2} \in \mathbb{R}$, and $\Phi : (g, \mathbf{x}) \in (\mathbb{Z}/2\mathbb{Z}) \times \mathbb{R}^2 \longrightarrow \mathbb{R}^2$ the action defined by $\phi(\overline{1}, \mathbf{x}) = s(\mathbf{x}) := (x_2, x_1)$, the symmetrized point of $\mathbf{x} = (x_1, x_2)$ with respect to the first bisector. The process S obtained by symmetrization of Y's restriction to $A = \{\mathbf{x} \in \mathbb{R}^2 : x_1 \leq x_2\}$ is defined by $S_{\mathbf{x}} = \frac{1}{1+\mathbf{1}_{\{\mathbf{x}\in\mathbb{R}^2 : s(\mathbf{x})=\mathbf{x}\}}(\mathbf{x})} Y_{\mathbf{x}} \mathbf{1}_A(\mathbf{x}) + \frac{1}{1+\mathbf{1}_{\{\mathbf{x}\in\mathbb{R}^2 : s(\mathbf{x})=\mathbf{x}\}}(\mathbf{x})} Y_{\mathbf{x}} \mathbf{1}_A(s(\mathbf{x}))$.*

The following example illustrates the fact that a random field which paths are almost sureley non-invariant under Φ may possess a modification which paths are all invariant under Φ:

Example 3. *Let $\Omega =]0, 1[$, $\mathcal{A} = \mathcal{B}(]0, 1[)$, $\mathbb{P}$ be Lebesgue's measure on Ω, $D = \mathbb{R}$, $G = \{e, s_0\}$ (s_0 be the symmetry with respect to 0), $F : x \in \mathbb{R} \longrightarrow \int_{-\infty}^{x} \frac{e^{-\frac{u^2}{2}}}{\sqrt{2\pi}} du \in]0, 1[$, $\varepsilon : \omega \in \Omega \longrightarrow \varepsilon(\omega) = F^{-1}(\omega) \in \mathbb{R}$, and $Y : (x, \omega) \in E \times \Omega \longrightarrow Y_x(\omega) = |x|\varepsilon(\omega)\mathbf{1}_{x \neq \varepsilon(\omega)}$. The process defined by $\widetilde{Y}_x(\omega) = |x|\varepsilon(\omega)$ has clearly all its paths invariant by s_0, and $\widetilde{Y}$ is a modification of Y since $\forall x \in D$, $P(Y_x = \tilde{Y}_x) = P(\varepsilon \neq x) = 1$. However, $\left\{\omega \in \Omega \ / \ (\forall x \in D,\ Y_x(\omega) = \tilde{Y}_x(\omega))\right\} = \left\{\frac{1}{2}\right\}$ is negligible, and the two processes are hence not indistinguable.*

Example 4. *Let us come back to the notations of example 2. One can construct a process having its paths invariant under Φ based on the process Y by defining $\forall \mathbf{x} \in D,\ Y^{\Phi}_{\mathbf{x}} = \frac{1}{2}(Y_{\mathbf{x}} + Y_{s(\mathbf{x})}) = \frac{1}{2}(Y_{(x_1,x_2)} + Y_{(x_2,x_1)})$. The covariance kernel of this new process Y^{Φ} is given by*

$$
\begin{aligned}
k_{X^{\Phi}}(x, x') &= \frac{1}{4}[k_X(x - x') + k_X(s(x) - x') + k_X(x - s(x')) + k_X(s(x) - s(x'))] \\
&= \frac{1}{4} e^{-||(x_1 - x'_1, x_2 - x'_2)||^2} + \frac{1}{4} e^{-||(x_1 - x'_1, x'_2 - x_2)||^2} + \frac{1}{4} e^{-||(x'_1 - x_1, x_2 - x'_2)||^2} \\
&+ \frac{1}{4} e^{-||(x'_1 - x_1, x'_2 - x_2)||^2}
\end{aligned}
\tag{13}
$$

3.2. **Kriging with an argumentwise invariant kernel.** Let us now come back to our prediction problem of origin, and assume that we dispose of n noiseless observations $Y_{\mathbf{x}_i} = y_i$ $(1 \leq i \leq n)$ of a squared-integrable centered random field $(Y_{\mathbf{x}})_{\mathbf{x} \in D}$ assumed invariant under the action Φ of a finite group

G on D. As recalled in the introduction (eq.1), the function

$$m : \mathbf{x} \in D \longrightarrow m(\mathbf{x}) = \mathbf{k}(\mathbf{x})' K^{-1} \mathbf{y},$$

is the Simple Kriging predictor (or "Kriging mean") of Y knowing the reponses at design points $\mathbf{x}_1, \ldots, \mathbf{x}_n$. In addition, the Simple Kriging variance (or "Mean Squared Error") s^2 is often used as a quantifyer of m's accuracy:

$$s^2 : \mathbf{x} \in D \longrightarrow s^2(\mathbf{x}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})' K^{-1} \mathbf{k}(\mathbf{x}). \tag{14}$$

It is well known that m interpolates the observations and s^2 vanishes at the design of experiments. As we will see now, more can be said in the case where k is argumentwise invariant.

Property 3.2. *(Properties of m and s^2 when k is argumentwise invariant)*

(1) *m and s^2 are invariant*

(2) $\forall i \in \{1, \ldots, n\}, \ \forall g \in G, \ m(g.\mathbf{x}_i) = y_i$ *and* $s^2(g.\mathbf{x}_i) = 0.$

Proof. (1) By argumentwise invariance of k, it is clear that the covariance vector $\mathbf{k}(.)$ is invariant as well. Pluging in the equality $\mathbf{k}(g.\mathbf{x}) = \mathbf{k}(\mathbf{x})$ in eqs 1 and 14, it follows that m and s^2 are invariant.

(2) Relies on (1) in the cases where $\mathbf{x} = g.\mathbf{x}_i$ $(i \in \{1, \ldots, n\})$.

□

In order to generalize to the conditional distribution of Y knowing $Y_{\mathbf{x}_i} = y_i$ $(1 \leq i \leq n)$, we can start by looking at its conditional covariance:

$$Cov(Y_{\mathbf{x}}, Y_{\mathbf{x}'} | Y_{\mathbf{X}} = \mathbf{y}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})' K^{-1} \mathbf{k}(\mathbf{x}'). \tag{15}$$

In the case where Y is assumed Gaussian, the Simple Kriging mean and variance at $\mathbf{x}$ coincide respectively with the conditional expectation and variance of $Y_{\mathbf{x}}$ knowing the observations. In addition, the Gaussian assumption makes it possible to get conditional simulations of Y, relying only on the conditional mean function and covariance kernel. The following property will play a crucial role in the applications of the next section.

Property 3.3. *(Properties of the conditional distribution of a Gaussian Random Field with argumentwise invariant kernel)*

(1) *The conditional random field has an argumentwise invariant kernel*

(2) *All conditional simulations are invariant*

Proof. (1) Follows from the invariance of $\mathbf{k}(.)$ applied to eq. 15.

(2) Both conditional expectation and conditional covariance being invariant, the conditional field is the sum of an invariant function with a centered field having an argumentwise invariant kernel. The paths of this field (up to a modification) are then invariant.

□

Remark 2. *In practice, the paths of Y are often simulated at a finite set of points $\mathbf{X}_{simu} = \{x_1, ..., x_m\} \subset D$ based on a matrix decomposition (Cholesky, Mahalanobis) of $K = (k_Y(x_i, x_j))_{1 \leq i,j \leq m}$. The invariance under Φ of the vectors simulated that way is thus sure (i.e. $\forall \omega \in \Omega$).*

3.3. **What about the RKHS point of view?** If k is argumentwise invariant and $\mathcal{H}$ is a RKHS of real-valued functions with kernel k, it is clear that any function $f \in \mathcal{H}$ is invariant under Φ. Indeed, taking any arbitrary $\mathbf{x} \in D$ and $g \in G$, we get

$$\begin{aligned} f(g.\mathbf{x}) &= \langle f, k(g.\mathbf{x}, .) \rangle_{\mathcal{H}} \\ &= \langle f, k(\mathbf{x}, .) \rangle_{\mathcal{H}} = f(\mathbf{x}) \end{aligned} \tag{16}$$

It clearly appears from that representation that the left invariance is sufficient. This is of course related to the fact that work here with symmetric kernels in the first place (in the sense that $k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}', \mathbf{x})$).

For the reciprocal, assuming that any $f \in \mathcal{H}$ is invariant, it is straightforward that all $k(\mathbf{x}, .)$'s ($\mathbf{x} \in D$) are invariant since they belong to $\mathcal{H}$.

Note that the case wher Mercer theorem applies is particularly enlightening. k then possesses an orthogonal expansion of the form

$$k(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{+\infty} \lambda_i e_i(\mathbf{x}) e_i(\mathbf{x}') \tag{17}$$

where the eigenfunctions $e_i(.)$ form an orthonormal basis of $L^2(D)$. Since the $e_i(.)$'s are in the RKHS, they are invariant, and it appears then in a very natural way that k is coordinatewise invariant.

4. Applications

4.1. Invariant Brownian Motion and other elementary examples.

4.1.1. *Symmetrized BM and OU process.* Let us first consider $(B_t)_{t \in [0, +\infty[}$, a one-dimensional Brownian Motion (BM), and the symmetry with respect to the origin $s : x \in D \longrightarrow -x \in D$, where $D := \mathbb{R}$. The corresponding action of the group $G = \mathbb{Z}/2\mathbb{Z}$ on $\mathbb{R}$ is the same as in Ex. 1. In order to symmetrize B, let us first extend it to a process on the whole line by setting $\forall t < 0,\ B_t = 0$. Now, relying on the fundamental domain $A := [0, +\infty[$, a straightforward way to symmetrize B is to construct B^{sym1} as follows:

$$B_t^{\text{sym1}} = B_{\pi_A(t)} = B_{|t|} \tag{18}$$

The resulting process is still centered and gaussian, with covariance

$$k_{B^{\text{sym1}}}(s,t) := Cov(B_s^{\text{sym1}}, B_t^{\text{sym1}}) = Cov(B_{|s|}, B_{|t|}) = \min(|s|, |t|) \tag{19}$$

Now, as we have seen in Ex. 4, another way of getting a process with symmetric paths based on B is by averaging it over the action's orbits:

$$B_t^{\text{sym2}} = \frac{1}{2}(B_t + B_{s(t)}) = \frac{1}{2}(B_t + B_{-t}) \tag{20}$$

Interestingly, this new process possesses the following covariance kernel:

$$\begin{aligned} k_{B^{\mathrm{sym2}}}(s,t) &:= Cov(B_s^{\mathrm{sym2}}, B_t^{\mathrm{sym2}}) \\ &= \frac{1}{4} Cov(B_s + B_{-s}, B_t + B_{-t}) = \frac{1}{4}\min(|s|,|t|), \end{aligned} \tag{21}$$

so that $k_{B^{\mathrm{sym2}}} = \frac{1}{4} k_{B^{\mathrm{sym1}}}$. Simulated paths of the centered Gaussian process defined by eq. 19 are represented on figure 1.

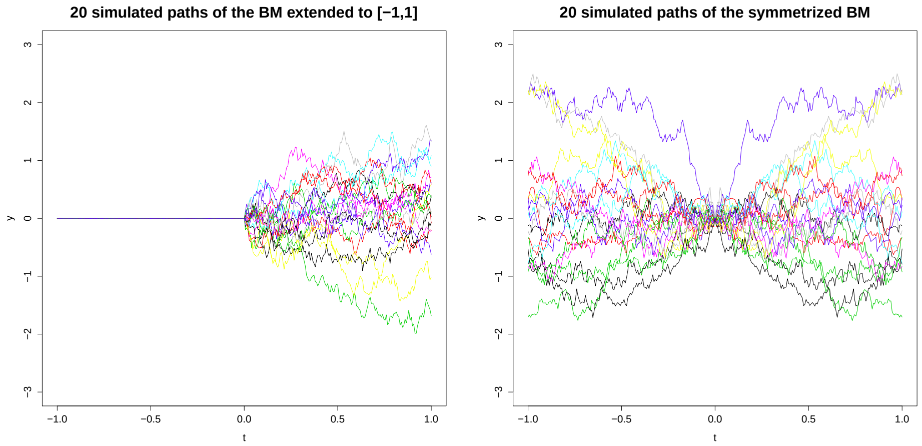

FIGURE 1. Symmetrization of the Brownian Motion relying on the symmetrized kernel (by projection on a fundamental domain) of eq. 19.

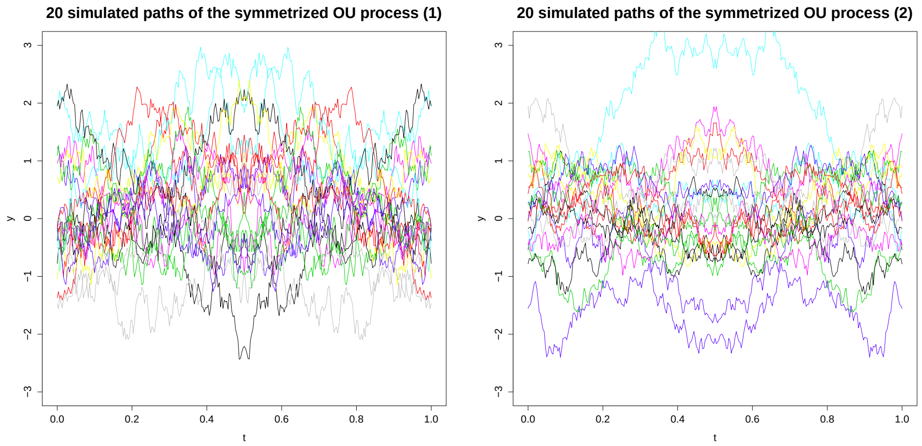

FIGURE 2. Symmetrization of the OU process relying on both kernels defined by eqs. 23, 25. Left: by projection on a fundamental domain (eq. 23). Right: by averaging over the orbits (eq. 25).

Let us now consider an Orstein-Uhlenbeck (OU) process $(Y_x)_{t\in D}$ restricted to $D := [0,1]$, and $s : t \in D \longrightarrow 1-t \in D$ the symmetry with respect to $\frac{1}{2}$. This time, we choose $A := [0, \frac{1}{2}]$ as fundamental domain. A similar construction as for the first symmetrized BM leads to the process

$$Y_t^{\text{sym1}} = Y_{\pi_A(t)} = Y_{\min(t,s(t))} = Y_{\min(t,1-t)} \tag{22}$$

This centered Gaussian process is then characterized by the kernel

$$\begin{aligned} k_{Y^{\text{sym1}}}(s,t) &:= Cov(Y_{\min(s,1-s)}, Y_{\min(t,1-t)}) \\ &= \exp\left(-|\min(s,1-s) - \min(t,1-t)|\right) \end{aligned} \tag{23}$$

On the other hand, the second symmetrized OU process is obtained by averaging over the orbits of the considered group action:

$$Y_t^{\text{sym2}} = \frac{1}{2}(Y_t + Y_{s(t)}) = \frac{1}{2}(Y_t + Y_{1-t}), \tag{24}$$

and possesses the following covariance kernel:

$$\begin{aligned} k_{Y^{\text{sym2}}}(s,t) &= \frac{1}{4} Cov(Y_s + Y_{1-s}, Y_t + Y_{1-t}) \\ &= \frac{1}{4}\exp\left(-|s-t|\right) + \frac{1}{4}\exp\left(-|(1-s)-t|\right) \\ &+ \frac{1}{4}\exp\left(-|s-(1-t)|\right) + \frac{1}{4}\exp\left(-|(1-s)-(1-t)|\right) \\ &= \frac{1}{2}\exp\left(-|s-t|\right) + \frac{1}{2}\exp\left(-|1-s-t|\right) \end{aligned} \tag{25}$$

Simulated paths of the centered Gaussian process defined by both eq. 23 and eq. 25 are represented on figure 2.

4.1.2. *Conditional simulations of an invariant Gaussian Process.* We now assume that the invariant process Y^{sym2} was observed at the 3 points $t_1 = 0.6, t_2 = 0.8, t_3 = 1$, with response values $y_1 = -0.8, y_2 = 0.5, y_3 = 0.9$. The covariance kernel of eq. 25 is used for performing simulations of Y^{sym2} conditionally on the latter observations. 20 such conditional simulations are represented on figure 3. As can be seen on figure 3, all paths are interpolating the conditioning data, illustrating the property 3.3 of the conditional distribution of Gaussian Random Fields with argumentwise invariant kernel.

4.2. **Kriging with an invariant kernel.** Let us finally apply Kriging with an argumentwise invariant kernel to a benchmark example from the structural reliability literature exhibiting obvious symmetries.

Quoting [7] in which this test-case was recently used, "the example has been analyzed by [41] and [15] made a comparison with several meta-models proposed by [36]". The limit state function of interest reads:

$$y : (x_1, x_2) \in [-5,5]^2 \longrightarrow \min \left\{ \begin{array}{l} 3 + 0.1(x_1 - x_2)^2 - (x_1 + x_2)/\sqrt{2} \\ 3 + 0.1(x_1 - x_2)^2 + (x_1 + x_2)/\sqrt{2} \\ (x_1 - x_2) + 6/\sqrt{2} \\ (x_1 - x_2) + 6/\sqrt{2} \end{array} \right\}$$

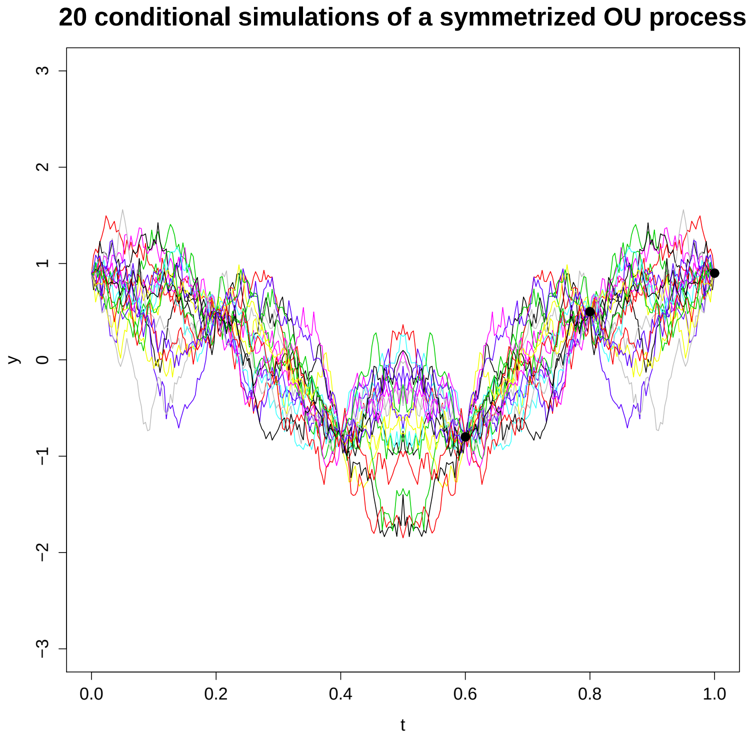

FIGURE 3. Conditional Simulations of the symmetrized OU process with the kernel of eq. 25. The black points stand for the conditioning data.

Figure 4 shows the contours of y, with an illustration of the three transformations of $\mathbb{R}^2$ –denoted by s_1, s_2, s_3– leaving y invariant.
Actually, y can be shown to be left invariant by an action of the group $(\mathbb{Z}/2\mathbb{Z})^2$ on $\mathbb{R}^2$. Indeed, as illustrated on figure 4, y is invariant under s_1, the axial symmetry with respect to the first bisector. y is also invariant under s_2, the axial symmetry with respect to the second bisector. Finally, y is naturally invariant under their composition, s_3, i.e. the symmetry with respect to the origin. Together with the identity of $\mathbb{R}^2$, denoted by s_0, the latter s_1, s_2, s_3 forms a group of order 4, representing $(\mathbb{Z}/2\mathbb{Z})^2$ on $\mathbb{R}^2$.

4.2.1. *Kriging with three different kernels.* Here we investigate using argumentwise invariant kernels for approximating this function by Ordinary Kriging based on 30 observations at a maximin LHS Design $\mathbf{X}$. The underlying Design of Experiments is generated using the R package *lhs*. As a preliminary step towards a comparison between different kernels, a Simple Kriging model with a tensor product OU kernel

$$k_Y(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left(-\frac{1}{\theta}\left(|x_1 - x_1'| + |x_2 - x_2'|\right)\right) + \tau^2 \mathbf{1}_{\mathbf{x}=\mathbf{x}'} \qquad (26)$$

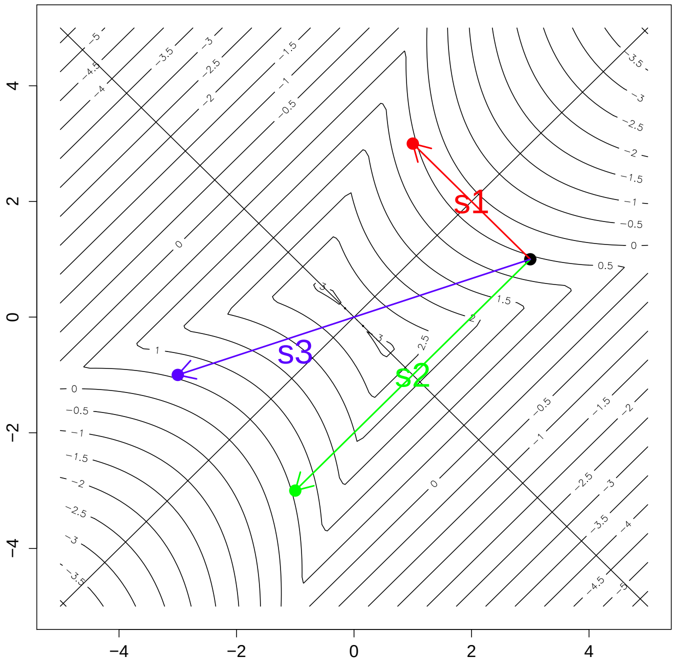

FIGURE 4. Borri and Speranzini's function, with its two axes of symmetry (black lines). The colored arrows stand for the three non-trivial transformations leaving this function unchanged.

is fitted to the data (see figure 5). Here the parameter are fixed to their Maximum Likelihood estimates, $\sigma^2 = 7.5$ and $\theta = 20$. In addition, a nugget effect with $\tau^2 = 0.01$ is added to k_Y for numerical purposes.
We now consider two different argumentwise invariant kernels. To start with, using similar notations as for the 1-dimensional OU example, we define a fundamental domain for Φ (see figure 6 for an illustration):

$$A := \{\mathbf{x} \in [-5, 5]^2 : x_1 \geq 0, -x_1 < x_2 \leq x_1\} \tag{27}$$

The first argumentwise invariant kernel considered is then constructed based on the projector $\pi_A : \mathbf{x} \in D \longrightarrow \pi_A(\mathbf{x}) = \mathcal{O}(\mathbf{x}) \cap A \in A$, as follows:

$$k_{Y^{\mathrm{sym1}}}(\mathbf{x}, \mathbf{x}') := k_Y(\pi_A(\mathbf{x}), \pi_A(\mathbf{x}')) \tag{28}$$

The second argumentwise invariant kernel considered is then constructed by averaging k_Y over the orbits of Φ:

$$k_{Y^{\mathrm{sym2}}}(\mathbf{x}, \mathbf{x}') := \frac{1}{16} \sum_{i=0}^{3} \sum_{j=0}^{3} k_Y(s_i.\mathbf{x}, s_j.\mathbf{x}') \tag{29}$$

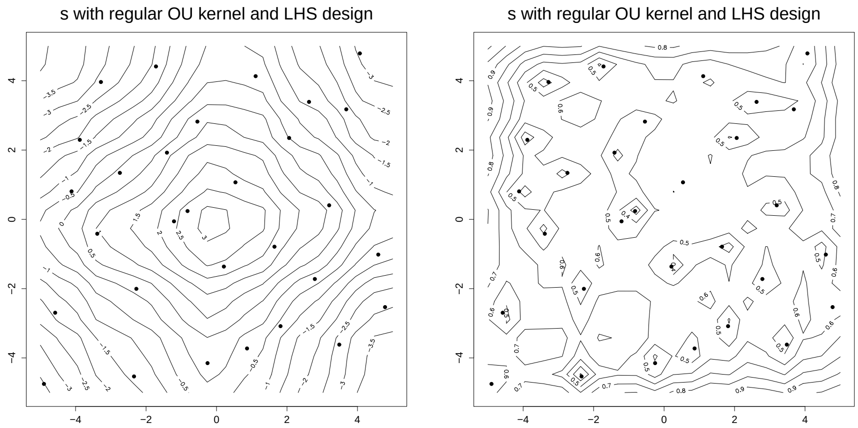

FIGURE 5. Simple Kriging mean and standard deviation with the regular tensor product kernel of eq. 26, based on observations of y at $\mathbf{X}$.

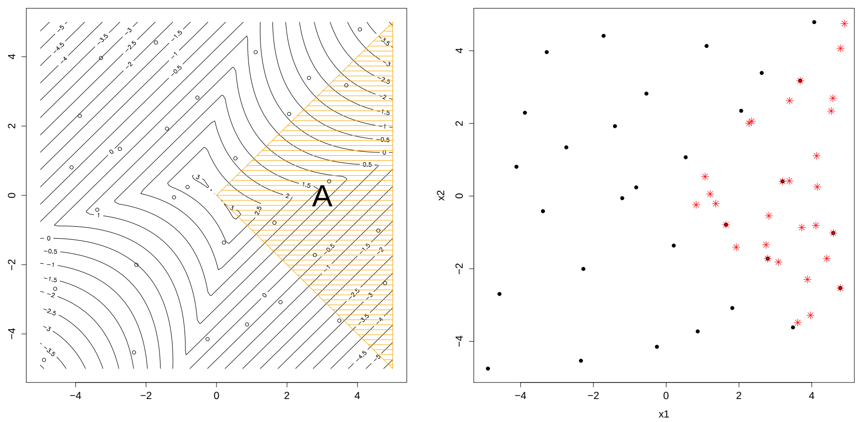

FIGURE 6. Left: the fundamental domain A for the considered action of $(\mathbb{Z}/2\mathbb{Z})^2$ on $[-5,5]^2$. The lower left boundary is excluded. Right: projection of the design points of $\mathbf{X}$ (black points) onto A (red stars).

The results of Kriging with kernels $k_{Y^{\text{sym1}}}$ and $k_{Y^{\text{sym2}}}$ based on the observations at $\mathbf{X}$ are illustrated on figures 7 and 8, respectively.

Finally, for comparison, a Kriging model with regular OU kernel (the same as for the first model) but based on the design

$$\mathbf{X}_{sym} := \bigcup_{i=0}^{3} s_i.\mathbf{X} \tag{30}$$

and with the observations at $\mathbf{X}$ replicated four times is considered.

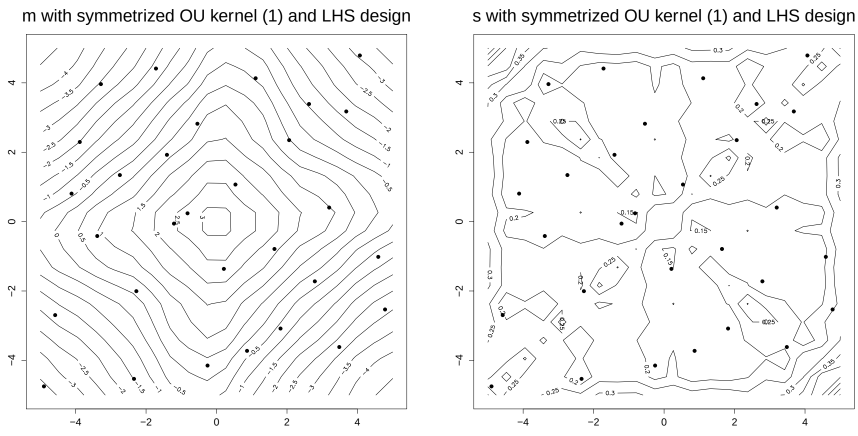

FIGURE 7. Simple Kriging mean and standard deviation with the symmetrized OU kernel of eq. 28, based on observations of y at $\mathbf{X}$.

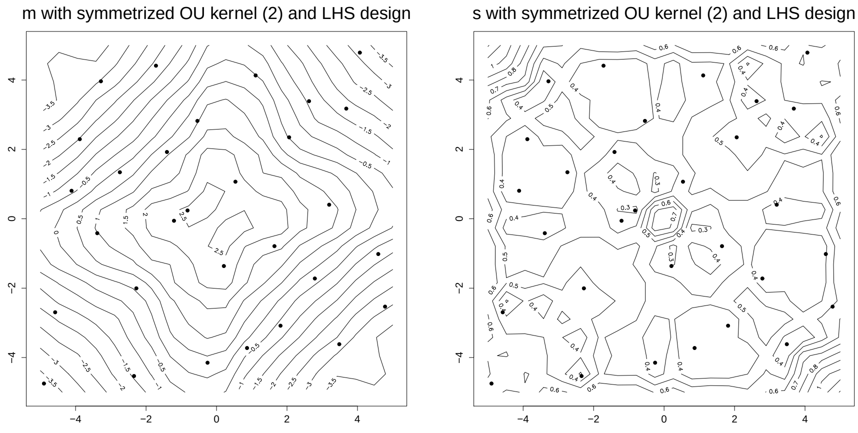

FIGURE 8. Simple Kriging mean and standard deviation with the symmetrized OU kernel of eq. 29, based on observations of y at $\mathbf{X}$.

4.2.2. *Discussion on the compared results.* In order to compare the prediction abilities of the four considered Kriging models, we predict y at a 50×50 out-of-sample validation design $\mathbf{X}_{val}$ using everyone of them, and compare the average prediction errors and the residuals. The graphics on figure 10 represent the mean predictions against reality (first line) and the standardized residuals (i.e. divided by the Kriging standard deviations, second line).

Looking at the values of the Integrated Squared Error (ISE) at $\mathbf{X}_{val}$ for the four candidate Kriging models, we first see that the first model is undoubtly dominated by the three other ones. This was to be expected since the first

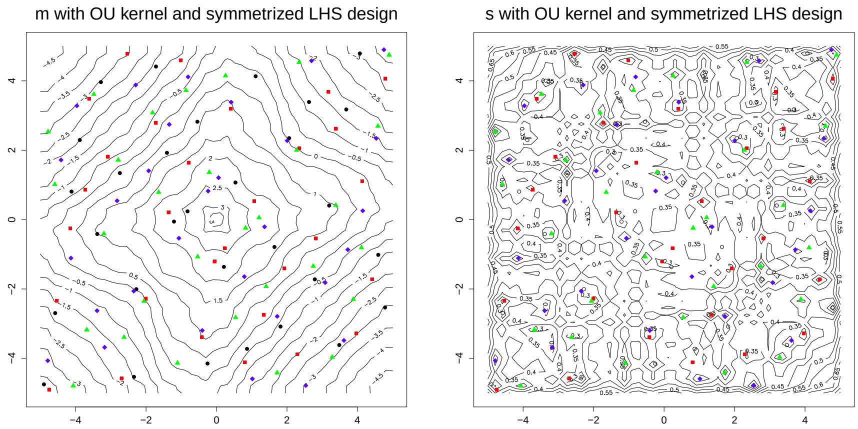

FIGURE 9. Simple Kriging mean and standard deviation with the regular tensor product kernel of eq. 26, based on observations of y at $\mathbf{X}_{sym}$. The solid black circles represent the LHS design $\mathbf{X}$. The red squares, blue diamonds, and green triangles represent respectively the orbits of $\mathbf{X}$ under the transformations s_1, s_2, and s_3.

model is the only one which doesn't take into account the symmetry of the problem. The second model, based on a combination of the OU kernel with the projector onto the fundamental domain of figure 6, shows significantly better performances. Indeed, the ISE drops from 433.01 to 264.33, just by playing on the underlying kernel. However, the performances of the third model, with the kernel averaged over the action's orbits, are even better. Not only does the ISE drop to 142.89, but the order of magnitude of the standardized residuals is more in accordance with what one usually expects when Kriging under the Gaussian Process assumption (even if this is not really theoretically well-founded, without further ergodicity assumptions, it is customary to expect that about 95% of the sample of standardized residuals lie between the 2.5% and 97.5% quantiles of the Gaussian distribution).

Perhaps surprisingly, the last model obtained by using a regular covariance kernel with a symmetrized design gave here better performances in terms of ISE (124.53) than the two previous models with argumentwise invariant kernels. This has to be tempered by the fact that doing it this way multplies the dimension of the covariance matrix by the order of the group (i.e. 4 here), that is to say that the total number of coefficients jumps from n^2 to $n^2 \times r^2$ (i.e. from 900 to $14'400$ here). Hence, replicating the design is likely to cause problems in terms of matrix inversion, and even in terms of data storage (for the reasonable values $n = 1000$ and $r = 8$, $n^2 \times r^2 = 64'000'000$). Furthermore, the test function studied here is not very smooth (so that an OU kernel was considered instead of a Gauss or a Matérn, more commonly used in smoother cases), which may relatively hinder the benefits of taking symmetries into account, since the latter come in more regular cases with

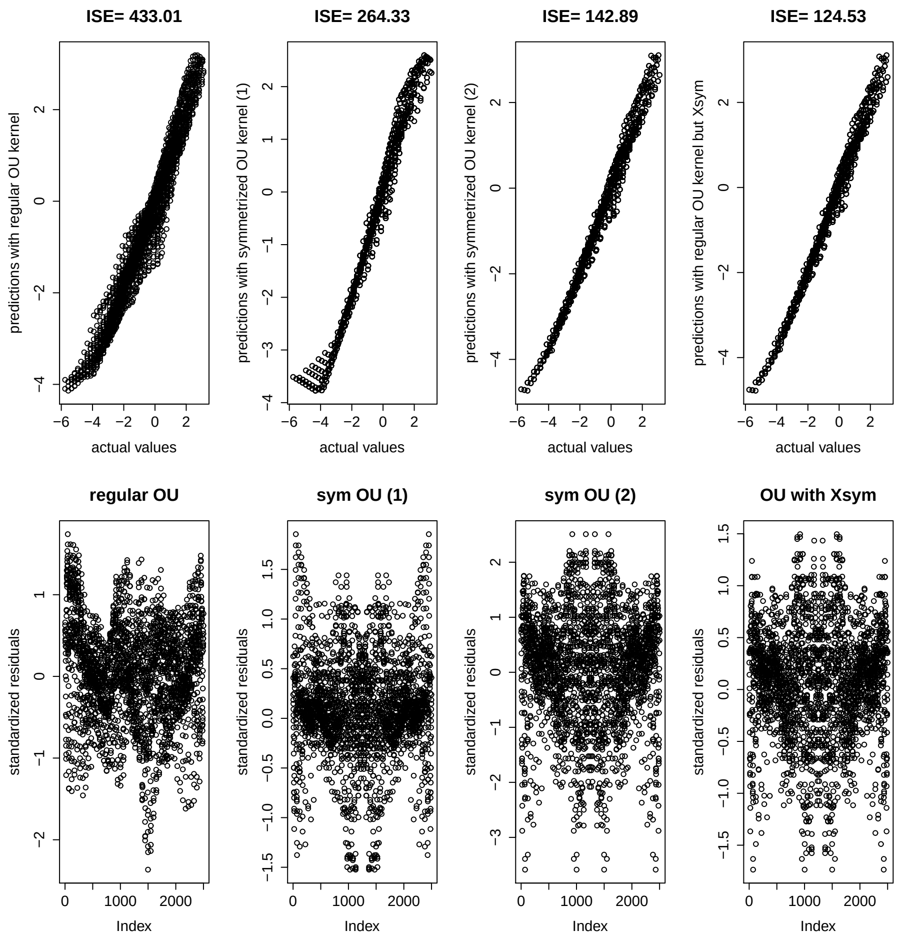

FIGURE 10. Comparison of prediction results at $\mathbf{X}_{val}$ when using the 4 Kriging models considered for Borri and Speranzini's function.

additional smoothness properties on the axes of symmetry. Concerning the second model, let us also remark that the choice of A is arbitrary, and not always without consequences on the model obtained. In the case of an anisotropic covariance, for instance, choosing the current A or its image by a rotation of center $\mathbf{0}$ and angle $\frac{\pi}{2}$ may lead to substantially different predictions. This has to be studied in more detail in further works.

To finish with this application, let us point out the fact that amon the considered models, only the ones based on an argumentwise invariant covariance kernel enables conditional simulations with invariant paths. 4 such simulated paths with the kernel of eq. 28 conditional on the observations at $\mathbf{X}$ are represented on figure 11.

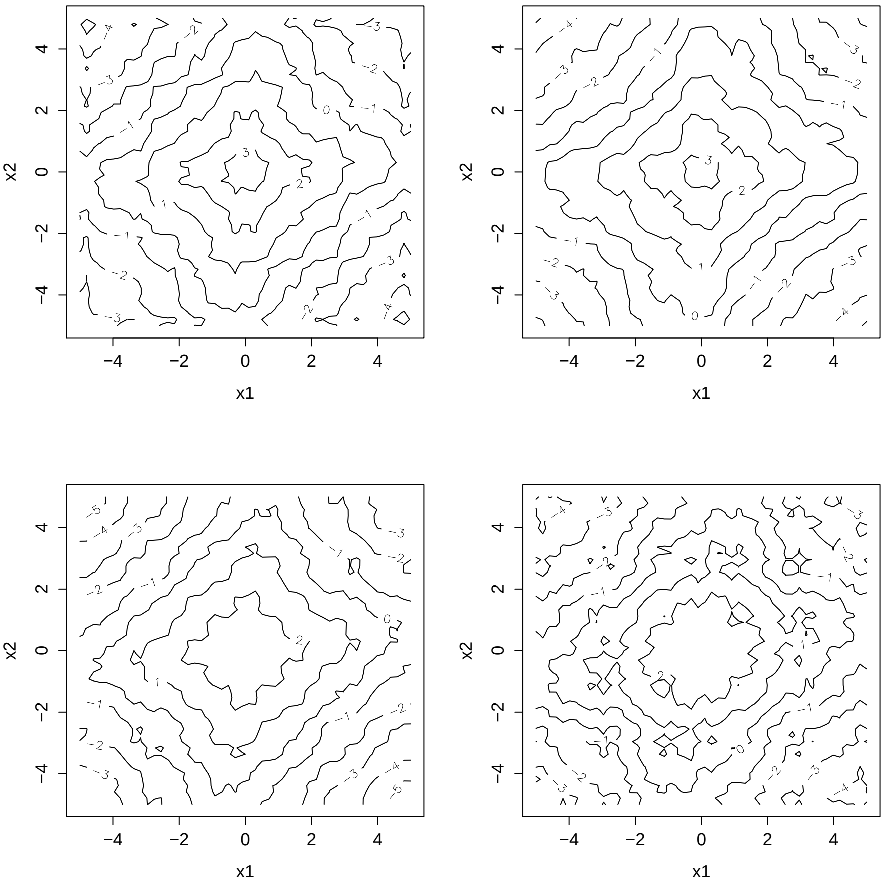

Figure 11. Four conditional simulations of Borri and Speranzini's function with symmetrized OU kernel (1), based on observations at $\mathbf{X}$.

5. Conclusion and perspectives

We proposed a class of covariance kernels, called *argumentwise invariant kernels*, characterizing (up to a modification) squared integrable random fields with invariant paths under an arbitrary action of a finite group on the index set, as well as reproducing kernel hilbert spaces of invariant functions (still with a finite group acting on the source space).

These kernels can be used for different purposes. We focused here on modeling invariant functions by Kriging. As discussed along the paper, Kriging models with an argumentwise invariant kernel have interesting properties, including the invariance of both Kriging mean and variance functions, but also the invariance of paths emanating from conditional simulations.

Among the two variants for making up invariant kernels based on arbitrary kernels proposed in the last example, summing a kernel over the orbits of the considered group action gave more convincing results than composing the basis kernel with a projection onto a fundamental domain. However, this may not hold in the general case, and further works may focus on identifying and unlocking the potential weak points of both considered approaches.

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