

# Equivalence of measures and asymptotically optimal linear prediction for Gaussian random fields with fractional-order covariance operators

DAVID BOLIN<sup>1,a</sup> and KRISTIN KIRCHNER<sup>2,b</sup>

<sup>1</sup>*CEMSE Division, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia,*

<sup>a</sup>*david.bolin@kaust.edu.sa*

<sup>2</sup>*Delft Institute of Applied Mathematics, Delft University of Technology, Delft, The Netherlands,*

<sup>b</sup>*k.kirchner@tudelft.nl*

We consider two Gaussian measures  $\mu, \tilde{\mu}$  on a separable Hilbert space, with fractional-order covariance operators  $A^{-2\beta}$  and  $\tilde{A}^{-2\tilde{\beta}}$ , respectively, and derive necessary and sufficient conditions on  $A, \tilde{A}$  and  $\beta, \tilde{\beta} > 0$  for I. equivalence of the measures  $\mu$  and  $\tilde{\mu}$ , and II. uniform asymptotic optimality of linear predictions for  $\mu$  based on the misspecified measure  $\tilde{\mu}$ . These results hold, e.g., for Gaussian processes on compact metric spaces. As an important special case, we consider the class of generalized Whittle–Matérn Gaussian random fields, where  $A$  and  $\tilde{A}$  are elliptic second-order differential operators, formulated on a bounded Euclidean domain  $\mathcal{D} \subset \mathbb{R}^d$  and augmented with homogeneous Dirichlet boundary conditions. Our outcomes explain why the predictive performances of stationary and non-stationary models in spatial statistics often are comparable, and provide a crucial first step in deriving consistency results for parameter estimation of generalized Whittle–Matérn fields.

*Keywords:* Gaussian measures; kriging; elliptic differential operators; Whittle–Matérn fields

## 1. Introduction and preliminaries

### 1.1. Introduction

Equivalence and orthogonality of Gaussian measures are essential concepts for investigating asymptotic properties of Gaussian random fields and stochastic processes. For example, they play a crucial role when proving consistency of maximum likelihood estimators for covariance parameters under infill asymptotics [2,34], or asymptotic optimality of linear predictions for random fields based on misspecified covariance models [30]. However, for the latter equivalence of the Gaussian measures is not a necessary assumption. This is an immediate consequence of the *necessary and sufficient* conditions for uniformly asymptotically optimal linear prediction, derived recently in [22] for Gaussian random fields on compact metric spaces. Both the necessary and sufficient conditions for equivalence of Gaussian measures as given by the Feldman–Hájek theorem [13, Theorem 2.25] and those for uniformly asymptotically optimal linear prediction [22, Assumption 3.3] are formulated in terms of the covariance operators rather than the covariance functions. Therefore, they may be difficult to verify. To the best of our knowledge there are not even *sufficient* conditions for asymptotic optimality available, which are easily verifiable, except for a few special cases such as stationary random fields on  $\mathbb{R}^d$ , see e.g. [28,29].

In the present work we remedy this lack. By means of complex interpolation theory combined with operator theory for fractional powers of closed operators, we are able to characterize the necessary and sufficient conditions mentioned above for a wide class of stationary and non-stationary Gaussian

processes. Specifically, in the first part we consider Gaussian measures on a generic separable Hilbert space with fractional-order covariance operators and translate the conditions of the Feldman–Hájek theorem (see Theorem B.1 in Appendix B) and of [22, Assumption 3.3] on the covariance operators  $A^{-2\beta}$ ,  $\tilde{A}^{-2\tilde{\beta}}$  to conditions on the non-fractional base operators  $A, \tilde{A}$ .

Our results are applicable to Gaussian random fields on compact metric spaces. As an important special case, we detail our outcomes for the class of generalized Whittle–Matérn Gaussian random fields [7,12,23]. The Matérn covariance family [26] is highly popular in spatial statistics and machine learning, see e.g. [19,27]. Given the parameters  $\nu, \sigma^2, \kappa > 0$ , which determine the smoothness, the variance, and the practical correlation range, respectively, the corresponding Matérn covariance function is

$$\varrho(s, s') = \varrho_0(\|s - s'\|_{\mathbb{R}^d}), \quad s, s' \in \mathbb{R}^d, \quad \text{where} \quad \varrho_0(h) := \frac{\sigma^2}{2\nu-1\Gamma(\nu)} (\kappa h)^\nu K_\nu(\kappa h). \tag{1.1}$$

Whittle [33] showed that the stationary solution  $Z: \mathbb{R}^d \times \Omega \rightarrow \mathbb{R}$  to the stochastic partial differential equation (SPDE for short)

$$(-\Delta + \kappa^2)^\beta Z = \mathcal{W} \quad \text{in } \mathbb{R}^d, \tag{1.2}$$

has covariance (1.1) with range parameter  $\kappa$ , smoothness  $\nu = 2\beta - d/2$ , and variance

$$\sigma^2 = (4\pi)^{-d/2} \kappa^{-2\nu} (\Gamma(\nu)/\Gamma(\nu + d/2)). \tag{1.3}$$

In the SPDE (1.2)  $\Delta$  is the Laplacian (see Appendix A.1.1),  $\beta > d/4$ , and  $\mathcal{W}$  is Gaussian white noise.

Motivated by this SPDE representation, Lindgren, Rue and Lindström [23] suggested extensions of the Matérn model to non-stationary models and to more general spatial domains. This has initiated an active research area, where spatial models based on SPDEs are proposed and investigated, see e.g. [4,10,16,21]. Most of the extensions that have been considered are special cases of *generalized Whittle–Matérn* Gaussian random fields, which are defined through fractional-order SPDEs of the form

$$(-\nabla \cdot (\mathbf{a}\nabla) + \kappa^2)^\beta Z = \mathcal{W} \quad \text{in } \mathcal{D}, \tag{1.4}$$

where  $\mathcal{D} \subset \mathbb{R}^d$  is a bounded Euclidean domain with boundary  $\partial\mathcal{D}$ ,  $\kappa: \mathcal{D} \rightarrow \mathbb{R}$  is a bounded real-valued function,  $\mathbf{a}: \mathcal{D} \rightarrow \mathbb{R}^{d \times d}$  is a (sufficiently nice) positive matrix-valued function, and  $\beta \in (d/4, \infty)$ . The fractional power  $L^\beta$  of the differential operator  $L = -\nabla \cdot (\mathbf{a}\nabla) + \kappa^2$  is understood in the spectral sense, where first  $L$  is augmented with appropriate boundary conditions on  $\partial\mathcal{D}$  (usually, homogeneous Dirichlet or Neumann conditions, see Appendix A.3). For this class of models,  $\kappa$  determines the *local* correlation ranges, whereas  $\mathbf{a}$  describes *local anisotropies*, see e.g. [16]. Whenever  $\kappa$  is constant and  $\mathbf{a}$  is the identity matrix, the model (1.4) reduces to the *classical* Whittle–Matérn model (1.2) on  $\mathcal{D} \subset \mathbb{R}^d$ .

Some properties of generalized Whittle–Matérn fields have already been discussed in the literature [8,9,12,20], but there are still considerably more results available for the original Gaussian Matérn class on  $\mathbb{R}^d$ . In particular, Zhang [34] and Anderes [2] investigated parameter estimation for Gaussian Matérn fields on  $\mathbb{R}^d$  under infill asymptotics. Thereby they showed that two Gaussian measures  $\mu_d(0; \nu, \sigma^2, \kappa)$  and  $\mu_d(0; \nu, \tilde{\sigma}^2, \tilde{\kappa})$ , corresponding to zero-mean Gaussian Matérn fields on  $\mathbb{R}^d$  with parameters  $\nu, \sigma^2, \kappa > 0$  and  $\nu, \tilde{\sigma}^2, \tilde{\kappa} > 0$ , respectively, are equivalent if and only if

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

Until now, the case  $d = 4$  has remained open. Furthermore, by [30, Theorem 12 in Chapter 4]  $\mu_d(0; \tilde{\nu}, \tilde{\sigma}^2, \tilde{\kappa})$  provides uniformly asymptotically optimal linear prediction for  $\mu_d(0; \nu, \sigma^2, \kappa)$  in any dimension  $d \in \mathbb{N}$  if  $\nu = \tilde{\nu}$ . Neither equivalence of measures nor asymptotic optimality of linear prediction have been characterized for generalized Whittle–Matérn fields yet.

Based on our general results for Gaussian measures with fractional-order covariance operators on a separable Hilbert space, combined with regularity theory for elliptic second-order partial differential equations, we are able to fill this gap in the second part of this work. Assuming that the coefficients  $\mathbf{a}, \tilde{\mathbf{a}}, \kappa, \tilde{\kappa}$  are smooth and that  $\mathcal{D} \subset \mathbb{R}^d$  has a smooth boundary  $\partial\mathcal{D}$ , we consider two Gaussian measures  $\mu_d(0; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(0; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  corresponding to generalized Whittle–Matérn fields (1.4) (using homogeneous Dirichlet boundary conditions on  $\partial\mathcal{D}$ ) with parameters  $(\beta, \mathbf{a}, \kappa)$  and  $(\tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , respectively. For this setting, we prove the following:

- I. In dimension  $d \leq 3$ ,  $\mu_d(0; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(0; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  are equivalent if and only if  $\beta = \tilde{\beta}$ ,  $\mathbf{a} = \tilde{\mathbf{a}}$  in  $\overline{\mathcal{D}}$ , and  $\tilde{\kappa}^2 - \kappa^2$  satisfies certain boundary conditions on  $\partial\mathcal{D}$ . In contrast, for  $d \geq 4$ , the measures are equivalent if and only if  $\beta = \tilde{\beta}$  and  $\mathbf{a} = \tilde{\mathbf{a}}$ ,  $\kappa^2 = \tilde{\kappa}^2$  in  $\overline{\mathcal{D}}$ .
- II. In any dimension  $d \in \mathbb{N}$ , the model  $\mu_d(0; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  provides uniformly asymptotically optimal linear prediction for the model  $\mu_d(0; \beta, \mathbf{a}, \kappa)$  if and only if  $\beta = \tilde{\beta}$ ,  $c\mathbf{a} = \tilde{\mathbf{a}}$  in  $\overline{\mathcal{D}}$  holds for some  $c \in (0, \infty)$ , and  $\tilde{\kappa}^2 - c\kappa^2$  fulfills certain boundary conditions on  $\partial\mathcal{D}$ .

These results cover the parameter range  $\beta \in (d/4, \infty) \setminus \{k + 1/4 : k \in \mathbb{N}\}$  and, in particular, also the case  $d = 4$  for the classical Matérn model (when considered on a bounded domain). Moreover, to the best of our knowledge these are the first explicit results on equivalence of measures and asymptotic efficiency of linear predictions for this general class of models. Outcome I. readily implies that, for  $d \leq 3$ , one cannot estimate all parameters of a generalized Whittle–Matérn field consistently, and it provides a crucial first step towards showing consistency of maximum likelihood estimates for the parameters  $\beta, \mathbf{a}$ . Result II. explains the comparable predictive performance of non-stationary and stationary models that has been noted for example in [16].

The outline is as follows: In the next subsection we introduce preliminaries and our notation. Section 2 is concerned with the general case of Gaussian measures on Hilbert spaces with fractional-order covariance operators. These outcomes are applied, in Section 3, to some first examples including the classical Whittle–Matérn model on a bounded domain  $\mathcal{D} \subset \mathbb{R}^d$  and, in Section 4, to derive the results I., II. for generalized Whittle–Matérn fields. In Section 5 the result II. is verified in two simulation studies for non-stationary random fields on the unit interval. Section 6 concludes with a discussion, and the Supplementary Material [6] contains six appendices (Appendix A/B/C/D/E/F) of the article.

### 1.2. Preliminaries and notation

If not specified otherwise,  $(\cdot, \cdot)_E$  denotes the inner product on a Hilbert space  $E$ ,  $\|\cdot\|_E$  the induced norm,  $\text{Id}_E$  the identity on  $E$ , and  $\mathcal{B}(E)$  the Borel  $\sigma$ -algebra on  $(E, \|\cdot\|_E)$ , that is the smallest  $\sigma$ -algebra containing all open sets. The scalar field  $\mathbb{K}$  is either given by the real numbers  $\mathbb{R}$  or the complex numbers  $\mathbb{C}$ . The dual  $E^*$  of  $E$  is the space containing all continuous linear functionals  $f: E \rightarrow \mathbb{K}$ , and we call  $\langle \cdot, \cdot \rangle: E^* \times E \rightarrow \mathbb{K}$ ,  $\langle f, \psi \rangle := f(\psi)$  the duality pairing between  $E^*$  and  $E$ .

The space of all bounded linear operators from  $(E, (\cdot, \cdot)_E)$  to a second Hilbert space  $(F, (\cdot, \cdot)_F)$  is denoted by  $\mathcal{L}(E; F)$ . It is rendered a Banach space when equipped with the usual operator norm  $\|T\|_{\mathcal{L}(E; F)} := \sup_{\psi \in E \setminus \{0\}} \frac{\|T\psi\|_F}{\|\psi\|_E}$ . We call a linear operator  $T: E \rightarrow F$  an isomorphism if  $T \in \mathcal{L}(E; F)$  and  $T^{-1} \in \mathcal{L}(F; E)$ , i.e.,  $T$  is bounded and has a bounded inverse. If  $V$  is a vector space such that  $E, F \subseteq V$  and if, in addition,  $\text{Id}_V|_E \in \mathcal{L}(E; F)$ , then  $E$  is continuously embedded in  $F$  and we write  $(E, \|\cdot\|_E) \hookrightarrow (F, \|\cdot\|_F)$ . The notation  $(E, \|\cdot\|_E) \cong (F, \|\cdot\|_F)$  indicates that  $(E, \|\cdot\|_E)$  and  $(F, \|\cdot\|_F)$  are isomorphic, i.e.,  $(E, \|\cdot\|_E) \hookrightarrow (F, \|\cdot\|_F) \hookrightarrow (E, \|\cdot\|_E)$ . Whenever  $E = F$ , we abbreviate  $\mathcal{L}(E) := \mathcal{L}(E; E)$ , and this convention holds also for all other spaces of operators to be introduced. The subspaces  $\mathcal{K}(E; F) \subseteq \mathcal{L}(E; F)$  and  $\mathcal{L}_2(E; F) \subseteq \mathcal{L}(E; F)$  contain all compact operators and Hilbert–Schmidt operators, respectively. Note that  $T \in \mathcal{L}(E; F)$  is compact if and only if it is

the limit in  $\mathcal{L}(E; F)$  of finite-rank operators, and  $\mathcal{L}_2(E; F)$  is a Hilbert space with the inner product  $(T, S)_{\mathcal{L}_2(E; F)} := \sum_{j \in \mathbb{N}} (Te_j, Se_j)_F$ , where  $\{e_j\}_{j \in \mathbb{N}}$  is any orthonormal basis for  $E$ . The adjoint of  $T \in \mathcal{L}(E; F)$  is identified with  $T^* \in \mathcal{L}(F; E)$  (via the Riesz maps on  $E$  and on  $F$ ). An operator  $T \in \mathcal{L}(E)$  is said to be orthogonal if  $TT^* = T^*T = \text{Id}_E$ , self-adjoint if  $T = T^*$ , nonnegative definite if  $(T\psi, \psi)_E \geq 0$  holds for all  $\psi \in E$ , and positive definite if there exists a constant  $\theta \in (0, \infty)$  such that  $(T\psi, \psi)_E \geq \theta \|\psi\|_E^2$  for all  $\psi \in E$ . A self-adjoint, nonnegative definite operator  $T \in \mathcal{L}(E)$  has a finite trace if  $\sum_{j \in \mathbb{N}} (Te_j, e_j)_E < \infty$  holds for an (or, equivalently, any) orthonormal basis  $\{e_j\}_{j \in \mathbb{N}}$  of  $E$ .

A (possibly unbounded) linear operator  $A$  on  $E$  with domain  $\mathcal{D}(A) = \{\psi \in E : \|A\psi\|_E < \infty\} \subseteq E$  is denoted by  $A: \mathcal{D}(A) \subseteq E \rightarrow E$ . It is closed if its graph  $\mathcal{G}(A) := \{(x, Ax) : x \in \mathcal{D}(A)\}$  is closed with respect to the norm  $\|(x, Ax)\|_{\mathcal{G}(A)} := \|x\|_E + \|Ax\|_E$  and densely defined if  $\mathcal{D}(A)$  is dense in  $E$ .

Throughout this article,  $(\Omega, \mathcal{F}, \mathbb{P})$  is a complete probability space. For a Hilbert space  $(E, (\cdot, \cdot)_E)$  and  $p \in [1, \infty)$ ,  $L_p(\Omega; E)$  denotes the space of (equivalence classes of)  $E$ -valued, Bochner measurable random variables with finite  $p$ -th moment, with norm  $\|Z\|_{L_p(\Omega; E)}^p := \int_{\Omega} \|Z(\omega)\|_E^p d\mathbb{P}(\omega)$ . Further,  $(X, d_X)$  is a connected, compact metric space of infinite cardinality, equipped with a strictly positive and finite Borel measure  $\nu_X$ , and  $L_2(X, \nu_X)$  is the Hilbert space of (equivalence classes of) real-valued, Borel measurable, square-integrable functions on  $X$ , with  $\|f\|_{L_2(X, \nu_X)}^2 := \int_X |f(x)|^2 d\nu_X(x)$ .

Finally, we write  $\mathbb{R}_+ := (0, \infty)$  for the positive part of the real axis,  $\mathbb{N}$  (or  $\mathbb{N}_0$ ) for the set of positive (respectively, nonnegative) integers, and  $\lfloor \cdot \rfloor$  (or  $\lceil \cdot \rceil$ ) for the floor (respectively, ceiling) function.

## 2. Gaussian processes with fractional-order covariance operators

Throughout this section we let  $(E, (\cdot, \cdot)_E)$  be a separable Hilbert space over  $\mathbb{R}$  with  $\dim(E) = \infty$ . Furthermore, we assume that  $\mu$  is a Gaussian measure on  $E$ , i.e., for every  $\psi \in E$ ,

$$\exists m_\psi \in \mathbb{R}, \sigma_\psi^2 \in \mathbb{R}_+ : \quad \forall B \in \mathcal{B}(\mathbb{R}) \quad \mu(\{\phi \in E : (\psi, \phi)_E \in B\}) = \mathbb{P}(\{\omega \in \Omega : z_\psi(\omega) \in B\}),$$

where  $z_\psi : \Omega \rightarrow \mathbb{R}$  is a random variable, which is either Gaussian distributed with mean  $m_\psi$  and variance  $\sigma_\psi^2$ , or concentrated at  $m_\psi$ , i.e.,  $\mathbb{P}(\{\omega \in \Omega : z_\psi(\omega) = m_\psi\}) = 1$ . Then, there exist a vector  $m \in E$  and a bounded linear operator  $C : E \rightarrow E$  such that, for all  $\psi, \psi' \in E$ ,

$$(m, \psi)_E = \int_E (\phi, \psi)_E d\mu(\phi), \quad (C\psi, \psi')_E = \int_E (\psi, \phi - m)_E (\phi - m, \psi')_E d\mu(\phi). \tag{2.1}$$

The vector  $m$  is the mean of the Gaussian measure  $\mu$  and  $C$  is its covariance operator. One can show that  $C : E \rightarrow E$  is self-adjoint, nonnegative definite, and has a finite trace [5, Theorem 2.3.1]. Moreover,  $\mu$  is uniquely determined by its mean  $m$  and its covariance operator  $C$ , and we therefore write  $\mu = \mathbf{N}(m, C)$ .

In this section we consider covariance operators of the form  $C = A^{-2\beta}$ , where  $A$  is an unbounded linear operator on  $E$  and  $\beta \in \mathbb{R}_+$ . The main objectives of this section are to characterize for two given Gaussian measures  $\mu := \mathbf{N}(m, A^{-2\beta})$  and  $\tilde{\mu} := \mathbf{N}(\tilde{m}, \tilde{A}^{-2\tilde{\beta}})$  the following:

- I. equivalence resp. orthogonality of  $\mu$  and  $\tilde{\mu}$ , see Subsection 2.2, and
- II. uniform asymptotic optimality of linear predictions for  $\mu$  based on the misspecified measure  $\tilde{\mu}$  when  $E = L_2(X, \nu_X)$ , see Subsection 2.3.

To this end, in Subsection 2.1 we first specify our assumptions on  $A$  and state two auxiliary results.

### 2.1. Hilbert space setting and some auxiliary results

In what follows, we assume that  $A : \mathcal{D}(A) \subseteq E \rightarrow E$  is a densely defined, self-adjoint, positive definite linear operator, which has a compact inverse  $A^{-1} \in \mathcal{K}(E)$ . In this case,  $A : \mathcal{D}(A) \subseteq E \rightarrow E$  is closed and

there exists an orthonormal basis  $\{e_j\}_{j \in \mathbb{N}}$  for  $E$  consisting of eigenvectors of  $A$ , with corresponding positive eigenvalues  $(\lambda_j)_{j \in \mathbb{N}}$  accumulating only at  $\infty$ . We assume that they are in non-decreasing order,  $0 < \lambda_1 \leq \lambda_2 \leq \dots$ , and repeated according to multiplicity.

For  $\beta \in [0, \infty)$ , the fractional power operator  $A^\beta : \mathcal{D}(A^\beta) \subseteq E \rightarrow E$  can then be defined using the spectral expansion

$$A^\beta \psi := \sum_{j \in \mathbb{N}} \lambda_j^\beta (\psi, e_j)_E e_j, \quad \psi \in \mathcal{D}(A^\beta) \subseteq E. \tag{2.2}$$

Note that, for all  $r \in [0, \infty)$ , the domain of the operator  $A^{r/2}$ ,

$$\dot{H}_A^r := \mathcal{D}(A^{r/2}), \quad \mathcal{D}(A^{r/2}) = \left\{ \psi \in E : \|A^{r/2} \psi\|_E^2 = \sum_{j \in \mathbb{N}} \lambda_j^r |(\psi, e_j)_E|^2 < \infty \right\}, \tag{2.3}$$

is itself a separable Hilbert space with respect to the inner product

$$(\phi, \psi)_{r,A} := (A^{r/2} \phi, A^{r/2} \psi)_E = \sum_{j \in \mathbb{N}} \lambda_j^r (\phi, e_j)_E (e_j, \psi)_E,$$

and the corresponding induced norm  $\|\cdot\|_{r,A}$ . Here,  $A^0 := \text{Id}_E$  and  $\dot{H}_A^0 := E$ . Recall that by definition the Cameron–Martin space of a Gaussian measure  $\mu = \mathcal{N}(m, C)$  on  $E$  (aka. the reproducing kernel Hilbert space of  $C$ ) is the image of  $E$  under  $C^{1/2}$ , endowed with the inner product  $(C^{-1/2} \cdot, C^{-1/2} \cdot)_E$ , cf. [5, p. 44]. It consists of all elements  $v \in E$  such that the measure  $\mu_v(B) := \mu(B - v)$  is absolutely continuous with respect to  $\mu$  (i.e.,  $\mu(B) = 0 \Rightarrow \mu_v(B) = 0$ ). In particular, for  $C = A^{-2\beta}$  we obtain that

$$C^{1/2}(E) = A^{-\beta}(E) = \mathcal{D}(A^\beta) = \dot{H}_A^{2\beta}, \quad \|C^{-1/2} \cdot\|_E = \|\cdot\|_{2\beta,A}. \tag{2.4}$$

We let  $\dot{H}_A^{-r}$  denote the dual space of  $\dot{H}_A^r$  after identification via the inner product on  $E$  which is continuously extended to a duality pairing. This means that for all  $\phi \in E \subseteq \dot{H}_A^{-r}$ ,  $\psi \in \dot{H}_A^r \subseteq E$ , we have that  $\langle \phi, \psi \rangle = (\phi, \psi)_E$ . It is an immediate consequence of these definitions that, for every  $r, \vartheta \in \mathbb{R}$ , the fractional power operator  $A^\vartheta : \dot{H}_A^r \rightarrow \dot{H}_A^{r-2\vartheta}$  is an isomorphism, possibly obtained as a continuous extension or restriction of  $A^\vartheta : \mathcal{D}(A^\vartheta) = \dot{H}_A^{2\vartheta} \rightarrow \dot{H}_A^0 = E$ . For ease of presentation, we postpone the technical proofs of the following two auxiliary results, Lemmas 2.1 and 2.2, to Appendix D.

**Lemma 2.1.** *Let  $A : \mathcal{D}(A) \subseteq E \rightarrow E$  and  $\tilde{A} : \mathcal{D}(\tilde{A}) \subseteq E \rightarrow E$  be two densely defined, self-adjoint, positive definite linear operators with compact inverses on  $E$ .*

- (i) *Assume that there exists  $\beta \in \mathbb{R}_+$  such that  $\tilde{A}^\beta A^{-\beta} : E \rightarrow E$  is an isomorphism and additionally  $A^{-\beta} \tilde{A}^{2\beta} A^{-\beta} - \text{Id}_E \in \mathcal{L}_2(E)$ . Then, for every  $\gamma \in [-\beta, \beta]$ , also the operator  $\tilde{A}^\gamma A^{-\gamma}$  is an isomorphism on  $E$  and  $A^{-\gamma} \tilde{A}^{2\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{L}_2(E)$ .*
- (ii) *Assume that there exists  $\beta \in \mathbb{R}_+$  such that  $\tilde{A}^\beta A^{-\beta} : E \rightarrow E$  is an isomorphism and additionally  $A^{-\beta} \tilde{A}^{2\beta} A^{-\beta} - \text{Id}_E \in \mathcal{K}(E)$ . Then, for every  $\gamma \in [-\beta, \beta]$ , also the operator  $\tilde{A}^\gamma A^{-\gamma}$  is an isomorphism on  $E$  and  $A^{-\gamma} \tilde{A}^{2\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{K}(E)$ .*

**Lemma 2.2.** *Let  $A : \mathcal{D}(A) \subseteq E \rightarrow E$  and  $\tilde{A} : \mathcal{D}(\tilde{A}) \subseteq E \rightarrow E$  be two densely defined, self-adjoint, positive definite linear operators with compact inverses on  $E$ , let  $\beta \in [1, \infty)$ , and define*

$$\mathfrak{N}_\beta := \{n \in \mathbb{N} : n \leq \beta\} \cup \{\beta\} = \{1, \dots, \lfloor \beta \rfloor\} \cup \{\beta\}. \tag{2.5}$$

- (i)  *$\tilde{A}^\gamma A^{-\gamma}$  is an isomorphism on  $E$  and  $A^{-\gamma} \tilde{A}^{2\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{L}_2(E)$  for all  $\gamma \in [-\beta, \beta]$  if and only if for all  $\eta \in \mathfrak{N}_\beta$  there exist an orthogonal operator  $U_\eta$  on  $E$  and  $S_\eta \in \mathcal{L}_2(E)$  such that  $\text{Id}_E + S_\eta$  is invertible on  $E$  and  $A^{\eta-1} \tilde{A} A^{-\eta} = U_\eta (\text{Id}_E + S_\eta)$ .*

- (ii)  $\widetilde{A}^\gamma A^{-\gamma}$  is an isomorphism on  $E$  and  $A^{-\gamma} \widetilde{A}^{2\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{K}(E)$  for all  $\gamma \in [-\beta, \beta]$  if and only if for every  $\eta \in \mathfrak{R}_\beta$  there exist an orthogonal operator  $W_\eta$  on  $E$  and  $K_\eta \in \mathcal{K}(E)$  such that  $\text{Id}_E + K_\eta$  is invertible on  $E$  and  $A^{\eta-1} \widetilde{A} A^{-\eta} = W_\eta(\text{Id}_E + K_\eta)$ .
- (iii) The linear operator  $\widetilde{A}^\gamma A^{-\gamma} : E \rightarrow E$  is an isomorphism for all  $\gamma \in [-\beta, \beta]$  if and only if  $\widetilde{A} - A \in \mathcal{L}(\dot{H}_A^{2\eta}; \dot{H}_A^{2(\eta-1)}) \cap \mathcal{L}(\dot{H}_A^{2\eta}; \dot{H}_A^{2(\eta-1)})$  holds for every  $\eta \in \{1, \beta\}$ .

## 2.2. Equivalence and orthogonality

Two probability measures  $\mu, \widetilde{\mu}$  on  $(E, \mathcal{B}(E))$  are said to be equivalent if, for all Borel sets  $B \in \mathcal{B}(E)$ ,  $\mu(B) = 0$  holds if and only if  $\widetilde{\mu}(B) = 0$ . In contrast, if there exists a Borel set  $B \in \mathcal{B}(E)$  such that  $\mu(B) = 0$  and  $\widetilde{\mu}(B) = 1$ , then  $\mu$  and  $\widetilde{\mu}$  are said to be orthogonal. Two Gaussian measures  $\mu, \widetilde{\mu}$  are either equivalent or orthogonal [5, Theorem 2.7.2]. As mentioned in the introduction, equivalence and orthogonality of Gaussian measures are important concepts in statistical theory. For example, a crucial first step in proving that a parameter  $\theta$  of a Gaussian process (with corresponding Gaussian measure  $\mu$ ) can be estimated consistently under infill asymptotics is often to define  $\widetilde{\mu}$  as the Gaussian measure corresponding to the process with parameter  $\theta \neq \theta$  and to show that  $\mu$  and  $\widetilde{\mu}$  are orthogonal, see [34].

The following proposition provides necessary and sufficient conditions for equivalence of two Gaussian measures  $\mu$  and  $\widetilde{\mu}$  when they have fractional-order covariance operators.

**Proposition 2.3.** *Let  $A : \mathcal{D}(A) \subseteq E \rightarrow E$  and  $\widetilde{A} : \mathcal{D}(\widetilde{A}) \subseteq E \rightarrow E$  be two densely defined, self-adjoint, positive definite linear operators with compact inverses on  $E$ . In addition, let  $\beta \in [1, \infty)$ ,  $\beta \in \mathbb{R}_+$  be such that  $A^{-2\beta}$  and  $\widetilde{A}^{-2\beta}$  have finite traces on  $E$ , let  $m, \widetilde{m} \in E$ , and define  $\delta := \beta/\beta \in \mathbb{R}_+$ . The Gaussian measures  $\mu = \mathcal{N}(m, A^{-2\beta})$  and  $\widetilde{\mu} = \mathcal{N}(\widetilde{m}, \widetilde{A}^{-2\beta})$  are either equivalent or orthogonal. They are equivalent if and only if the following two conditions are satisfied:*

- (a) the difference of the means satisfies  $m - \widetilde{m} \in \dot{H}_A^{2\beta}$ ;
- (b) for all  $\eta \in \mathfrak{R}_\beta$ , where  $\mathfrak{R}_\beta$  is defined as in (2.5), there exist an orthogonal operator  $U_\eta \in \mathcal{L}(E)$  and  $S_\eta \in \mathcal{L}_2(E)$  such that  $A^{\eta-1} \widetilde{A}^\delta A^{-\eta} = U_\eta(\text{Id}_E + S_\eta)$  and  $\text{Id}_E + S_\eta$  is invertible on  $E$ .

Condition (b) is in particular satisfied, whenever

$$\widetilde{A}^\delta - A \in \mathcal{L}_2(\dot{H}_A^{2\eta}; \dot{H}_A^{2(\eta-1)}) \quad \forall \eta \in \mathfrak{R}_\beta, \quad \text{and} \quad \widetilde{A}^\delta - A \in \mathcal{L}(\dot{H}_A^{2\delta\eta}; \dot{H}_A^{2\delta(\eta-1)}) \quad \forall \eta \in \{1, \beta\}.$$

**Proof.** In order to derive the equivalence statement, we apply the Feldman–Hájek theorem, see Theorem B.1 in Appendix B in the Supplementary Material [6]:  $\mu$  and  $\widetilde{\mu}$  are equivalent if and only if

- (i) the Cameron–Martin spaces  $\dot{H}_A^{2\beta}$  and  $\dot{H}_{\widetilde{A}}^{2\beta}$  (see (2.4)) are norm equivalent Hilbert spaces;
- (ii) the difference of the means satisfies  $m - \widetilde{m} \in \dot{H}_A^{2\beta}$ ; and
- (iii) the operator  $A^{-\beta} \widetilde{A}^{2\beta} A^{-\beta} - \text{Id}_E$  is a Hilbert–Schmidt operator on  $E$ .

It remains to prove that conditions (i) and (iii) are equivalent to condition (b) of the proposition. By Lemma 2.2(i), applied for the pair of operators  $A, \widetilde{A}^\delta$ , (b) is equivalent to  $(\widetilde{A}^\delta)^\gamma A^{-\gamma} = \widetilde{A}^{\delta\gamma} A^{-\gamma}$  being an isomorphism on  $E$  and  $A^{-\gamma} (\widetilde{A}^\delta)^{2\gamma} A^{-\gamma} - \text{Id}_E = A^{-\gamma} \widetilde{A}^{2\delta\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{L}_2(E)$  for  $\gamma \in [-\beta, \beta]$ . The choice  $\gamma := \beta$  shows that  $\dot{H}_A^{2\beta} \cong \dot{H}_{\widetilde{A}}^{2\beta}$  and  $A^{-\beta} \widetilde{A}^{2\beta} A^{-\beta} - \text{Id}_E \in \mathcal{L}_2(E)$ , i.e., (i) and (iii) hold. Conversely, if (i) and (iii) are satisfied, then by Lemma 2.1(i) we obtain that  $\widetilde{A}^{\delta\gamma} A^{-\gamma}$  is an isomorphism on  $E$  and  $A^{-\gamma} \widetilde{A}^{2\delta\gamma} A^{-\gamma} - \text{Id}_E \in \mathcal{L}_2(E)$  for all  $\gamma \in [-\beta, \beta]$ . Thus, (b) is satisfied by Lemma 2.2(i).

Since  $A^{\eta-1}\tilde{A}^\delta A^{-\eta} - \text{Id}_E = A^{\eta-1}(\tilde{A}^\delta - A)A^{-\eta}$ , the condition  $\tilde{A}^\delta - A \in \mathcal{L}_2(\dot{H}_A^{2\eta}; \dot{H}_A^{2(\eta-1)})$  implies that  $S_\eta := A^{\eta-1}\tilde{A}^\delta A^{-\eta} - \text{Id}_E \in \mathcal{L}_2(E)$  for all  $\eta \in \mathfrak{R}_\beta$ . Furthermore, if also  $\tilde{A}^\delta - A$  is in  $\mathcal{L}(\dot{H}_{\tilde{A}}^{2\delta\eta}; \dot{H}_{\tilde{A}}^{2\delta(\eta-1)}) = \mathcal{L}(\dot{H}_{\tilde{A}^\delta}^{2\eta}; \dot{H}_{\tilde{A}^\delta}^{2(\eta-1)})$  for  $\eta \in \{1, \beta\}$ , then by Lemma 2.2(iii) (applied for the pair of operators  $A, \tilde{A}^\delta$ )  $\tilde{A}^\delta A^{-\gamma}$  is an isomorphism on  $E$  for all  $\gamma \in [-\beta, \beta]$ . Therefore,  $\text{Id}_E + S_\eta = A^{\eta-1}\tilde{A}^{-\delta(\eta-1)}\tilde{A}^\delta A^{-\eta}$  is invertible on  $E$ , and (b) holds for the choice  $U_\eta = \text{Id}_E$  for all  $\eta \in \mathfrak{R}_\beta$ .  $\square$

By applying Proposition 2.3 for the pair of measures  $\hat{\mu} := \mathbf{N}(m, \tilde{A}^{-2})$  and  $\tilde{\mu} = \mathbf{N}(\tilde{m}, \tilde{A}^{-2\tilde{\beta}})$ , where  $\hat{A} := A^\beta$ , we also obtain a corresponding result which includes the case that  $\beta \in (0, 1)$ .

**Corollary 2.4.** *Under the assumptions of Proposition 2.3 on  $m, \tilde{m}, A, \tilde{A}$ , and for  $\beta, \tilde{\beta} \in \mathbb{R}_+$  such that  $A^{-2\beta}, \tilde{A}^{-2\tilde{\beta}}$  have finite traces, the Gaussian measures  $\mu = \mathbf{N}(m, A^{-2\beta})$  and  $\tilde{\mu} = \mathbf{N}(\tilde{m}, \tilde{A}^{-2\tilde{\beta}})$  are equivalent if and only if (a)  $m - \tilde{m} \in \dot{H}_A^{2\beta}$  and (b) there exist an orthogonal operator  $U \in \mathcal{L}(E)$  and  $S \in \mathcal{L}_2(E)$  such that  $\tilde{A}^{\tilde{\beta}}A^{-\beta} = U(\text{Id}_E + S)$  and  $\text{Id}_E + S$  is invertible on  $E$ .*

**Remark 2.5.** At first glance, condition (b) of Corollary 2.4 seems easier compared to (b) of Proposition 2.3. We note that the advantage of the latter is that, whenever  $\beta = \tilde{\beta}$ , it is formulated solely in terms of the base operator  $\tilde{A}$  (and not of powers thereof).

### 2.3. Uniformly asymptotically optimal linear prediction

Throughout this subsection, we let  $(X, d_X)$  be a connected, compact metric space with positive, finite Borel measure  $\nu_X$  (see Subsection 1.2) and we consider  $E = L_2(X, \nu_X)$ . Suppose that  $Z : X \times \Omega \rightarrow \mathbb{R}$  is a square-integrable random field with mean  $m \in L_2(X, \nu_X)$  and covariance operator  $A^{-2\beta}$ , where  $A : \mathcal{D}(A) \subseteq L_2(X, \nu_X) \rightarrow L_2(X, \nu_X)$  is as described in Subsection 2.1. Let  $\mu = \mathbf{N}(m, A^{-2\beta})$  be the Gaussian measure corresponding to  $Z$  and define  $\mathbb{E}[\cdot]$  as the expectation under  $\mu$ . That is, for a random variable  $Y : \Omega \rightarrow L_2(X, \nu_X)$  with distribution  $\mu$  and a Borel measurable function  $g : L_2(X, \nu_X) \rightarrow \mathbb{R}$ , we have that  $m = \mathbb{E}[Y] := \int_{L_2(X, \nu_X)} y \, d\mu(y)$  and, provided that the integral  $\int_{L_2(X, \nu_X)} g(y) \, d\mu(y)$  exists, we define  $\mathbb{E}[g(Y)] := \int_{L_2(X, \nu_X)} g(y) \, d\mu(y)$ .

To characterize optimal linear prediction for  $Z$ , we introduce the centered process  $Z^0 := Z - m$  and the vector space  $\mathcal{Z}^0$  consisting of all linear combinations of the form  $\alpha_1 Z^0(x_1) + \dots + \alpha_K Z^0(x_K)$ , where  $K \in \mathbb{N}$  and  $\alpha_j \in \mathbb{R}, x_j \in X$  for all  $j \in \{1, \dots, K\}$ . We then define the Hilbert space  $\mathcal{H}^0$  as the closure of  $\mathcal{Z}^0$  with respect to the norm  $\|\cdot\|_{\mathcal{H}^0}$  induced by the  $L_2(\Omega, \mathbb{P})$  inner product,

$$\left( \sum_{j=1}^K \alpha_j Z^0(x_j), \sum_{k=1}^{K'} \alpha'_k Z^0(x'_k) \right)_{\mathcal{H}^0} := \sum_{j=1}^K \sum_{k=1}^{K'} \alpha_j \alpha'_k \mathbb{E}[Z^0(x_j)Z^0(x'_k)].$$

Since any observation or linear predictor of  $Z$  can be represented as  $h = c + h^0$  for  $c \in \mathbb{R}$  and  $h^0 \in \mathcal{H}^0$ , we introduce the Hilbert space  $\mathcal{H}$  as the direct sum  $\mathcal{H} := \mathbb{R} \oplus \mathcal{H}^0$  equipped with the graph norm  $\|h\|_{\mathcal{H}}^2 = |c|^2 + \|h^0\|_{\mathcal{H}^0}^2$ . Suppose now that we want to predict  $h \in \mathcal{H}$  based on a set of observations  $\{y_{nj}\}_{j=1}^n$ , where  $y_{nj} = c_{nj} + y_{nj}^0$ , for  $c_{nj} \in \mathbb{R}$  and  $y_{nj}^0 \in \mathcal{H}^0$ . Then, the best linear predictor (also known as kriging predictor, see e.g. [30, Section 1.2] and [22, Section 2]) of  $h$  based on these observations is the  $\mathcal{H}$ -orthogonal projection of  $h$  onto the subspace

$$\mathcal{H}_n := \mathbb{R} \oplus \mathcal{H}_n^0 = \left\{ \alpha_0 + \sum_{j=1}^n \alpha_j y_{nj}^0 : \alpha_0, \dots, \alpha_n \in \mathbb{R} \right\}, \quad \mathcal{H}_n^0 := \text{span}\{y_{nj}^0\}_{j=1}^n. \tag{2.6}$$

That is, the best linear predictor  $h_n \in \mathcal{H}_n$  satisfies

$$(h_n - h, g_n)_{\mathcal{H}} = 0 \quad \forall g_n \in \mathcal{H}_n, \quad \text{and} \quad \|h_n - h\|_{\mathcal{H}} = \inf_{g_n \in \mathcal{H}_n} \|g_n - h\|_{\mathcal{H}}. \tag{2.7}$$

The question is now what happens if we replace  $h_n$  with another linear predictor  $\tilde{h}_n$ , which is computed based on an incorrect model. Specifically, let  $\tilde{\mu} = \mathbf{N}(\tilde{m}, \tilde{A}^{-2\tilde{\beta}})$  be a second Gaussian measure with corresponding expectation operator  $\tilde{\mathbb{E}}[\cdot]$ , and let  $\tilde{h}_n$  be the best linear predictor for the model  $\tilde{\mu}$ . We are interested in the quality of  $\tilde{h}_n$  compared to  $h_n$  asymptotically as  $n \rightarrow \infty$ . For this purpose, we assume that the set of observations  $\{y_{nj}\}_{j=1}^n : n \in \mathbb{N}\}$  yields  $\mu$ -consistent kriging prediction, i.e.,

$$\lim_{n \rightarrow \infty} \mathbb{E}[(h_n - h)^2] = \lim_{n \rightarrow \infty} \|h_n - h\|_{\mathcal{H}}^2 = 0, \tag{2.8}$$

and we let  $\mathcal{S}_{\text{adm}}^{\mu}$  denote the set of all admissible sequences of observations which provide  $\mu$ -consistent kriging prediction:

$$\begin{aligned} \mathcal{S}_{\text{adm}}^{\mu} := & \{ \{ \mathcal{H}_n \}_{n \in \mathbb{N}} \mid \forall n \in \mathbb{N} : \mathcal{H}_n \text{ is as in (2.6) with } \dim(\mathcal{H}_n^0) = n, \\ & \forall h \in \mathcal{H} : \{ h_n \}_{n \in \mathbb{N}} \text{ defined by (2.7) satisfy (2.8)} \}. \end{aligned} \tag{2.9}$$

By combining the results of Lemmas 2.1 and 2.2 with [22, Theorem 3.8] we obtain the following result on uniformly asymptotically optimal linear prediction when misspecifying  $\mu$  by  $\tilde{\mu}$ .

**Proposition 2.6.** *Let  $h_n$  and  $\tilde{h}_n$  denote the best linear predictors of  $h \in \mathcal{H}$  based on  $\mathcal{H}_n$  and the measures  $\mu = \mathbf{N}(m, A^{-2\beta})$  and  $\tilde{\mu} = \mathbf{N}(\tilde{m}, \tilde{A}^{-2\tilde{\beta}})$ , respectively. Here, we assume that  $m, \tilde{m} \in L_2(\mathcal{X}, \nu_{\mathcal{X}})$ ,  $A : \mathcal{D}(A) \subseteq L_2(\mathcal{X}, \nu_{\mathcal{X}}) \rightarrow L_2(\mathcal{X}, \nu_{\mathcal{X}})$  and  $\tilde{A} : \mathcal{D}(\tilde{A}) \subseteq L_2(\mathcal{X}, \nu_{\mathcal{X}}) \rightarrow L_2(\mathcal{X}, \nu_{\mathcal{X}})$  are densely defined, self-adjoint, positive definite linear operators with compact inverses on  $L_2(\mathcal{X}, \nu_{\mathcal{X}})$ . In addition,  $\beta, \tilde{\beta} \in \mathbb{R}_+$  are such that  $A^{-2\beta}$  and  $\tilde{A}^{-2\tilde{\beta}}$  have finite traces on  $L_2(\mathcal{X}, \nu_{\mathcal{X}})$  and  $\delta := \tilde{\beta}/\beta$ .*

I. Set  $\mathcal{H}_{-n} := \{ h \in \mathcal{H} : \mathbb{E}[(h_n - h)^2] > 0 \}$ . Any of the following four asymptotic statements,

$$\lim_{n \rightarrow \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\mathbb{E}[(\tilde{h}_n - h)^2]}{\mathbb{E}[(h_n - h)^2]} = 1, \quad \lim_{n \rightarrow \infty} \sup_{h \in \mathcal{H}_{-n}} \frac{\tilde{\mathbb{E}}[(h_n - h)^2]}{\tilde{\mathbb{E}}[(\tilde{h}_n - h)^2]} = 1, \tag{2.10}$$

$$\lim_{n \rightarrow \infty} \sup_{h \in \mathcal{H}_{-n}} \left| \frac{\tilde{\mathbb{E}}[(h_n - h)^2]}{\mathbb{E}[(h_n - h)^2]} - c \right| = 0, \quad \lim_{n \rightarrow \infty} \sup_{h \in \mathcal{H}_{-n}} \left| \frac{\mathbb{E}[(\tilde{h}_n - h)^2]}{\tilde{\mathbb{E}}[(\tilde{h}_n - h)^2]} - \frac{1}{c} \right| = 0, \tag{2.11}$$

holds for all  $\{ \mathcal{H}_n \}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^{\mu}$  (and in (2.11) for some  $c \in \mathbb{R}_+$ ) if and only if

- (a) the difference of the means satisfies  $m - \tilde{m} \in \dot{H}_A^{2\tilde{\beta}}$ ;
- (b) there exist  $c \in \mathbb{R}_+$ , an orthogonal operator  $W$  on  $L_2(\mathcal{X}, \nu_{\mathcal{X}})$ , and  $K \in \mathcal{K}(L_2(\mathcal{X}, \nu_{\mathcal{X}}))$  such that  $c^{1/2} \tilde{A}^{\tilde{\beta}} A^{-\beta} = W(\text{Id}_{L_2(\mathcal{X}, \nu_{\mathcal{X}})} + K)$  and  $\text{Id}_{L_2(\mathcal{X}, \nu_{\mathcal{X}})} + K$  is invertible.

In this case, the constant  $c \in \mathbb{R}_+$  in condition (b) coincides with that in (2.11).

II. For  $\beta \in [1, \infty)$ , condition (b) is equivalent to requiring that there exists  $c \in \mathbb{R}_+$  such that for all  $\eta \in \mathfrak{R}_{\beta}$ , where  $\mathfrak{R}_{\beta}$  is defined as in (2.5), there exist an orthogonal operator  $W_{\eta}$  on  $L_2(\mathcal{X}, \nu_{\mathcal{X}})$  and  $K_{\eta} \in \mathcal{K}(L_2(\mathcal{X}, \nu_{\mathcal{X}}))$  such that  $c^{\frac{1}{2\beta}} A^{\eta-1} \tilde{A}^{\tilde{\beta}} A^{-\eta} = W_{\eta}(\text{Id}_{L_2(\mathcal{X}, \nu_{\mathcal{X}})} + K_{\eta})$  and  $\text{Id}_{L_2(\mathcal{X}, \nu_{\mathcal{X}})} + K_{\eta}$  is invertible on  $L_2(\mathcal{X}, \nu_{\mathcal{X}})$ . This is satisfied, whenever the following holds:

$$\forall \eta \in \mathfrak{R}_{\beta} : \quad c^{\frac{1}{2\beta}} \tilde{A}^{\tilde{\beta}} - A \in \mathcal{K}(\dot{H}_A^{2\eta}; \dot{H}_A^{2(\eta-1)}) \cap \mathcal{L}(\dot{H}_A^{2\delta\eta}; \dot{H}_A^{2\delta(\eta-1)}).$$



**Proof.** By [22, Theorem 3.8 and Lemma B.1] any of the assertions in (2.10) or (2.11) holds for every  $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^\mu$  and for some constant  $c \in \mathbb{R}_+$  if and only if

- (i) the Cameron–Martin spaces  $\dot{H}_A^{2\beta}$  and  $\dot{H}_{\tilde{A}}^{2\beta}$  are norm equivalent Hilbert spaces;
- (ii) the difference of the means satisfies  $m - \tilde{m} \in \dot{H}_A^{2\beta}$ ; and
- (iii)  $A^{-\beta} \tilde{A}^{2\beta} A^{-\beta} - c^{-1} \text{Id}_E = c^{-1} (A^{-\beta} (c \tilde{A}^{2\beta}) A^{-\beta} - \text{Id}_E)$  is compact on  $E$ .

The proof for II., when  $\beta \in [1, \infty)$ , can then be completed as in the proof of Proposition 2.3, namely by using Lemma 2.1(ii) and Lemma 2.2(ii)/(iii) for the pair of operators  $A$  and  $c^{\frac{1}{2\beta}} \tilde{A}^\delta$ . Finally, the general statement I. for  $\beta, \tilde{\beta} \in \mathbb{R}_+$  follows similarly as Corollary 2.4. □

### 3. Some explicit choices for the base operators

In this section we illustrate the abstract results of Section 2 by two first examples before discussing their implications for generalized Whittle–Matérn fields in the next section: In Subsection 3.1 we consider the case that the base operators  $A$  and  $\tilde{A}$  diagonalize with respect to the same eigenbasis  $\{e_j\}_{j \in \mathbb{N}}$  for  $E$ . This setting applies to classical Whittle–Matérn fields with constant coefficients, which solve SPDEs of the form (1.2) on a bounded domain  $\mathcal{D} \subset \mathbb{R}^d$ . We subsequently discuss this example in Subsection 3.2.

#### 3.1. Operators with the same eigenbasis

We note that the scope for applications of the following corollary is considerably wider than the classical Whittle–Matérn class discussed in Subsection 3.2. For instance, it can be used for periodic random fields on  $\mathcal{X} = [0, 1]^d$  as considered by Stein [29], random fields on the sphere  $\mathcal{X} = \mathbb{S}^2$  defined via the spherical harmonics, see e.g. [18] and [22, Section 6.3], or more generally Gaussian processes on compact Riemannian manifolds defined via the eigenfunctions of the Laplace–Beltrami operator [11].

**Corollary 3.1.** *Let  $A: \mathcal{D}(A) \subseteq E \rightarrow E$  and  $\tilde{A}: \mathcal{D}(\tilde{A}) \subseteq E \rightarrow E$  be two densely defined, self-adjoint, positive definite linear operators with compact inverses on  $E$ . In addition, assume that  $A$  and  $\tilde{A}$  diagonalize with respect to the same eigenbasis  $\{e_j\}_{j \in \mathbb{N}}$  for  $E$ , i.e., there exist corresponding eigenvalues  $\mathbb{R}_+ \ni \lambda_j, \tilde{\lambda}_j \rightarrow \infty$  (as  $j \rightarrow \infty$ ) such that  $Ae_j = \lambda_j e_j$  and  $\tilde{A}e_j = \tilde{\lambda}_j e_j$  for all  $j \in \mathbb{N}$ . Let  $m, \tilde{m} \in E$ , and assume that  $\beta, \delta \in \mathbb{R}_+$  are such that  $A^{-2\beta}$  and  $\tilde{A}^{-2\delta\beta}$  have finite traces on  $E$ . Then, the Gaussian measures  $\mu = \mathbf{N}(m, A^{-2\beta})$  and  $\tilde{\mu} = \mathbf{N}(\tilde{m}, \tilde{A}^{-2\delta\beta})$  satisfy the following:*

- I. *The Cameron–Martin spaces for  $\mu$  and  $\tilde{\mu}$  are isomorphic, with equivalent norms, if and only if there exist  $c_-, c_+ \in \mathbb{R}_+$  such that  $c_j := \tilde{\lambda}_j^\delta \lambda_j^{-1} \in [c_-, c_+]$  for all  $j \in \mathbb{N}$ .*
- II. *The measures  $\mu$  and  $\tilde{\mu}$  are equivalent if and only if  $m - \tilde{m} \in \dot{H}_A^{2\beta}$  and  $\sum_{j \in \mathbb{N}} (c_j - 1)^2 < \infty$ .*
- III. *Any of the four assertions in (2.10), (2.11) holds for all  $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^\mu$  and in (2.11) for some  $c \in \mathbb{R}_+$  if and only if  $m - \tilde{m} \in \dot{H}_A^{2\beta}$  and  $\lim_{j \rightarrow \infty} c_j = \hat{c}$  for some  $\hat{c} \in \mathbb{R}_+$ . Then,  $c = \hat{c}^{-2\beta}$ .*

**Proof.** Define  $c_- := \inf_{j \in \mathbb{N}} \tilde{\lambda}_j^\delta \lambda_j^{-1} \in [0, \infty)$  and  $c_+ := \sup_{j \in \mathbb{N}} \tilde{\lambda}_j^\delta \lambda_j^{-1} \in (0, \infty]$ . Then, we obtain that  $\inf_{\phi \in \dot{H}_A^{2\beta}} \frac{\|\phi\|_{2\delta\beta, \tilde{A}}}{\|\phi\|_{2\beta, A}} = c_-^\beta$  and  $\sup_{\phi \in \dot{H}_A^{2\beta}} \frac{\|\phi\|_{2\delta\beta, \tilde{A}}}{\|\phi\|_{2\beta, A}} = c_+^\beta$ . Therefore, the Cameron–Martin spaces for  $\mu$  and  $\tilde{\mu}$ , see (2.4), are isomorphic if and only if  $c_- > 0$  and  $c_+ < \infty$ .

Note that  $(c_j)_{j \in \mathbb{N}} \subset \mathbb{R}_+$  and  $\sum_{j \in \mathbb{N}} (c_j - 1)^2 < \infty$  imply that  $0 < c_- \leq c_j \leq c_+ < \infty$  for all  $j \in \mathbb{N}$ . Thus, II. follows from I. and the Feldman–Hájek theorem since by the mean value theorem applied for

$t \mapsto t^{2\beta}$ , we have  $\|A^{-\beta} \widetilde{A}^{2\delta\beta} A^{-\beta} - \text{Id}_E\|_{\mathcal{L}_2(E)}^2 = \sum_{j \in \mathbb{N}} (c_j^{2\beta} - 1)^2 = 4\beta^2 \sum_{j \in \mathbb{N}} \xi_j^{2(2\beta-1)} (c_j - 1)^2$ , where the numbers  $(\xi_j)_{j \in \mathbb{N}}$  satisfy that  $\xi_j \in [\min\{c_j, 1\}, \max\{c_j, 1\}] \subseteq [\min\{c_-, 1\}, \max\{c_+, 1\}]$  for all  $j \in \mathbb{N}$ .

Finally, the assertion III. has already been observed in [22, Corollary 5.1]; there formulated in terms of the ratio  $\widetilde{\gamma}_j/\gamma_j \rightarrow c$  (as  $j \rightarrow \infty$ ) of the eigenvalues  $(\widetilde{\gamma}_j)_{j \in \mathbb{N}}$  and  $(\gamma_j)_{j \in \mathbb{N}}$  of the covariance operators  $\widetilde{C} = \widetilde{A}^{-2\delta\beta}$  and  $C = A^{-2\beta}$ . Thus,  $\widetilde{\gamma}_j/\gamma_j = \widetilde{\lambda}_j^{-2\delta\beta} \lambda_j^{2\beta} = c_j^{-2\beta}$  and the claim follows.  $\square$

**Remark 3.2.** Note that for  $\mu = \mathbf{N}(0, A^{-2\beta})$  and  $\widetilde{\mu} = \mathbf{N}(0, \widetilde{A}^{-2\delta\beta})$  the conditions in all parts of Corollary 3.1 are independent of  $\beta \in \mathbb{R}_+$ . This implies that once a property (equivalent Cameron–Martin spaces, equivalence of measures, or uniformly asymptotically optimal linear prediction) is established for  $\mu, \widetilde{\mu}$  and a fixed  $\beta = \beta_0 \in \mathbb{R}_+$ , it follows also for all other meaningful values of  $\beta \in \mathbb{R}_+$  so that  $A^{-2\beta}, \widetilde{A}^{-2\delta\beta}$  have finite traces. Thus, in the case that  $A$  and  $\widetilde{A}$  diagonalize with respect to the same eigenbasis, besides concluding the corresponding property for  $\beta \leq \beta_0$  (by means of Lemma 2.1) one obtains it also for  $\beta > \beta_0$ . This observation holds even for more general base operators  $A, \widetilde{A}$ . Specifically, if their fractional powers commute, i.e.,  $\mathcal{D}(\widetilde{A}^\vartheta A^r) = \mathcal{D}(A^r \widetilde{A}^\vartheta)$  and  $\widetilde{A}^\vartheta A^r \psi = A^r \widetilde{A}^\vartheta \psi$  for all  $r, \vartheta \in \mathbb{R}$  and  $\psi \in \mathcal{D}(\widetilde{A}^\vartheta A^r)$ , then the operators  $A^{\eta-1} \widetilde{A}^\delta A^{-\eta}$ ,  $\eta \in \mathfrak{N}_\beta$ , appearing in the conditions of Propositions 2.3 and 2.6 simplify to  $\widetilde{A}^\delta A^{-1}$  and the conditions become independent of  $\beta \in [1, \infty)$ .

### 3.2. Whittle–Matérn operators with constant coefficients

We now discuss classical Whittle–Matérn fields solving the SPDE (1.2) on a bounded domain. To this end, let  $\emptyset \neq \mathcal{D} \subset \mathbb{R}^d$  be a connected, bounded and open domain, with Lipschitz boundary  $\partial\mathcal{D}$ . Further,

$$Lv := (-\Delta + \kappa^2)v, \quad v \in \mathcal{D}(L) := H^2(\mathcal{D}) \cap H_0^1(\mathcal{D}), \tag{3.1}$$

is the negative Laplacian, shifted by  $\kappa^2 \in [0, \infty)$  and augmented with homogeneous Dirichlet boundary conditions, see Appendix A.3. By Proposition 4.2  $L^{-2\beta}$  has a finite trace if and only if  $\beta \in (d/4, \infty)$ . Recall that for the SPDE (1.2) on  $\mathbb{R}^d$  this condition corresponds to a positive smoothness parameter  $\nu = 2\beta - d/2 \in \mathbb{R}_+$ . For two classical Whittle–Matérn fields with parameters  $(\beta, \tau, \kappa)$  and  $(\widetilde{\beta}, \widetilde{\tau}, \widetilde{\kappa})$ , where  $\tau, \widetilde{\tau}$  scale the variances of the fields, cf. (5.1), we obtain the following result from Corollary 3.1.

**Corollary 3.3.** *Let  $d \in \mathbb{N}$ ,  $\beta, \widetilde{\beta} \in (d/4, \infty)$ ,  $\tau, \widetilde{\tau} \in \mathbb{R}_+$ , and let  $L, \widetilde{L}$  be defined as in (3.1) with shift parameters  $\kappa^2 \in [0, \infty)$  and  $\widetilde{\kappa}^2 \in [0, \infty)$ , respectively. Assume that  $m, \widetilde{m} \in L_2(\mathcal{D})$  and consider the Gaussian measures  $\mu = \mathbf{N}(m, \tau^{-2}L^{-2\beta})$  and  $\widetilde{\mu} = \mathbf{N}(\widetilde{m}, \widetilde{\tau}^{-2}\widetilde{L}^{-2\widetilde{\beta}})$  on the Hilbert space  $L_2(\mathcal{D})$ .*

- I. *The Cameron–Martin spaces for  $\mu$  and  $\widetilde{\mu}$  are isomorphic, with equivalent norms, if and only if  $\beta = \widetilde{\beta}$ .*
- II. *In dimension  $d \leq 3$ ,  $\mu$  and  $\widetilde{\mu}$  are equivalent if and only if  $\beta = \widetilde{\beta}$ ,  $\tau = \widetilde{\tau}$  and  $m - \widetilde{m} \in \dot{H}_L^{2\beta}$ . In dimension  $d \geq 4$ ,  $\mu$  and  $\widetilde{\mu}$  are equivalent if and only if  $\beta = \widetilde{\beta}$ ,  $\tau = \widetilde{\tau}$ ,  $m - \widetilde{m} \in \dot{H}_L^{2\beta}$  and  $\kappa^2 = \widetilde{\kappa}^2$ .*
- III. *In every dimension  $d \in \mathbb{N}$ , any of the four assertions in (2.10), (2.11) holds for every sequence  $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^\mu$  and in (2.11) for some  $c \in \mathbb{R}_+$  if and only if  $\beta = \widetilde{\beta}$  and  $m - \widetilde{m} \in \dot{H}_L^{2\beta}$ .*

**Proof.** Letting  $(\widehat{\lambda}_j)_{j \in \mathbb{N}}$  denote the eigenvalues of the negative Dirichlet Laplacian  $-\Delta$  with corresponding eigenfunctions  $\{e_j\}_{j \in \mathbb{N}}$  forming an orthonormal basis of  $L_2(\mathcal{D})$ , we find that  $\{e_j\}_{j \in \mathbb{N}}$  is also an eigenbasis for  $L$  and  $\widetilde{L}$ , with eigenvalues  $\lambda_j = \widehat{\lambda}_j + \kappa^2$  and  $\widetilde{\lambda}_j = \widehat{\lambda}_j + \widetilde{\kappa}^2$ , respectively. The asymptotic behavior  $\widehat{\lambda}_j \sim j^{2/d}$ , see (4.4), shows that  $c_j := \widetilde{\tau}^{1/\beta} \tau^{-1/\beta} \widetilde{\lambda}_j^\delta \lambda_j^{-1} \in [c_-, c_+]$  holds for some  $c_-, c_+ \in \mathbb{R}_+$  and all  $j \in \mathbb{N}$  if and only if  $\delta = \widetilde{\beta}/\beta = 1$ ; then,  $\lim_{j \rightarrow \infty} c_j = (\frac{\widetilde{\tau}}{\tau})^{1/\beta}$  so that  $\tau = \widetilde{\tau}$  is necessary for  $\mu \sim \widetilde{\mu}$ . Then,  $(c_j - 1)^2 \sim (\widetilde{\kappa}^2 - \kappa^2)^2 j^{-4/d}$  and all assertions follow from Corollary 3.1.  $\square$

## 4. Generalized Whittle–Matérn fields on Euclidean domains

Throughout this section, let  $\mathcal{D} \subset \mathbb{R}^d$  be a nonempty, connected, bounded and open domain with Lipschitz continuous boundary  $\partial\mathcal{D}$  (see Definition A.1 in Appendix A) and closure  $\overline{\mathcal{D}} = \mathcal{D} \cup \partial\mathcal{D}$ .

The purpose of this section is to generalize the results obtained in Corollary 3.3 for classical Whittle–Matérn fields to the class of generalized Whittle–Matérn fields (1.4) on  $\mathcal{D}$ , where  $\kappa$  and  $\mathbf{a}$  are functions describing spatially varying correlation ranges and anisotropies, respectively. The difficulty of this generalization lies in the fact that the covariance operators of two generalized Whittle–Matérn fields do not necessarily have the same eigenfunctions. For this reason, more sophisticated arguments and tools from spectral theory and PDE theory are needed. We refer to Appendix A for an overview of several important results from PDE theory and all relevant function spaces, such as the Lebesgue spaces  $L_p(\mathcal{D})$ ,  $L_p(\partial\mathcal{D})$ ,  $p \geq 1$ , the spaces of smooth functions  $C^\infty(\overline{\mathcal{D}})$  and  $C_c^\infty(\mathcal{D})$ , the (fractional-order) Sobolev spaces  $H^r(\mathcal{D})$  for  $r \in \mathbb{R}_+$ , and the subspace  $H_0^1(\mathcal{D}) \subset H^1(\mathcal{D})$ .

### 4.1. Setting and summary of the main results

In order to properly define the class of generalized Whittle–Matérn fields (1.4), we consider for  $\beta \in \mathbb{R}_+$  the fractional-order SPDE

$$L^\beta Z = \mathcal{W}, \quad \mathbb{P}\text{-almost surely}, \tag{4.1}$$

where  $\mathcal{W}$  denotes Gaussian white noise on the Hilbert space  $L_2(\mathcal{D})$ , and  $L^\beta$  is a (possibly fractional) power of an elliptic differential operator  $L$  which determines the covariance structure of the random field  $Z: \overline{\mathcal{D}} \times \Omega \rightarrow \mathbb{R}$ . Specifically, we assume that  $L: \mathcal{D}(L) \subseteq L_2(\mathcal{D}) \cap H_0^1(\mathcal{D}) \rightarrow L_2(\mathcal{D})$  is a linear, symmetric, second-order differential operator in divergence form with homogeneous Dirichlet boundary conditions (see Appendix A.3 in the Supplementary Material [6]), formally given by

$$Lv = -\nabla \cdot (\mathbf{a} \nabla v) + \kappa^2 v, \quad v \in \mathcal{D}(L) \subseteq L_2(\mathcal{D}) \cap H_0^1(\mathcal{D}). \tag{4.2}$$

Here, we suppose that  $\mathbf{a}$  and  $\kappa$  in (4.2) and the spatial domain  $\mathcal{D} \subset \mathbb{R}^d$  satisfy the following conditions.

**Assumption 4.1.**

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

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

In addition,  $\mathbf{a} = (\mathbf{a}_{jk})_{j,k=1}^d$  is smooth,  $\mathbf{a}_{jk} \in C^\infty(\overline{\mathcal{D}})$  for all  $j, k \in \{1, \dots, d\}$ .

II.  $\kappa: \overline{\mathcal{D}} \rightarrow \mathbb{R}$  is smooth,  $\kappa \in C^\infty(\overline{\mathcal{D}})$ .

III.  $\mathcal{D} \subset \mathbb{R}^d$  has a smooth boundary  $\partial\mathcal{D}$  of class  $C^\infty$ , see Definition A.1 in Appendix A.

Provided that Assumptions 4.1.I–II are satisfied, the differential operator  $L$  in (4.2) is strongly elliptic and induces a symmetric, continuous and coercive bilinear form on  $H_0^1(\mathcal{D})$ ,

$$a_L: H_0^1(\mathcal{D}) \times H_0^1(\mathcal{D}) \rightarrow \mathbb{R}, \quad a_L(u, v) := (\mathbf{a} \nabla u, \nabla v)_{L_2(\mathcal{D})} + (\kappa^2 u, v)_{L_2(\mathcal{D})}. \tag{4.3}$$

The domain of the operator  $L: \mathcal{D}(L) \subset L_2(\mathcal{D}) \rightarrow L_2(\mathcal{D})$  is given by  $\mathcal{D}(L) = H^2(\mathcal{D}) \cap H_0^1(\mathcal{D})$  and, in particular, we find that  $L$  is densely defined and self-adjoint. Furthermore, the Rellich–Kondrachov compactness theorem [1, Theorem 6.3] implies that  $L^{-1}: L_2(\mathcal{D}) \rightarrow H_0^1(\mathcal{D}) \subset L_2(\mathcal{D})$  is compact on  $L_2(\mathcal{D})$ , see Appendix A.3 for more details.

For this reason, there exists a countable system of eigenfunctions  $\{e_j\}_{j \in \mathbb{N}}$  of  $L$  which can be chosen as an orthonormal basis for  $L_2(\mathcal{D})$ . We assume that the corresponding positive eigenvalues  $(\lambda_j)_{j \in \mathbb{N}}$  are in non-decreasing order,  $0 < \lambda_1 \leq \lambda_2 \leq \dots$ , and repeated according to multiplicity. The fractional power operator  $L^\beta$  in the SPDE (4.1) is then defined in the spectral sense as in (2.2), with  $A := L$  and  $E := L_2(\mathcal{D})$ . Weyl’s law [14, Theorem 6.3.1] states that the eigenvalues  $(\lambda_j)_{j \in \mathbb{N}} \subset \mathbb{R}_+$  of the strongly elliptic second-order differential operator  $L$  satisfy the spectral asymptotics

$$\exists c_\lambda, C_\lambda \in \mathbb{R}_+ : \quad c_\lambda j^{2/d} \leq \lambda_j \leq C_\lambda j^{2/d} \quad \forall j \in \mathbb{N}. \tag{4.4}$$

Existence and uniqueness of the solution  $Z$  to (4.1) thus follow from [9, Proposition 2.3, Remark 2.4] or [12, Lemma 3]. We recapitulate this result in the next proposition.

**Proposition 4.2.** *For  $\mathcal{D} \subset \mathbb{R}^d$ ,  $d \in \mathbb{N}$ , let the differential operator  $L$  be as in (4.2), and suppose that  $\mathbf{a}$  and  $\kappa$  satisfy Assumptions 4.1.I–II. Then, the SPDE (4.1) has a unique solution  $Z \in L_p(\Omega; L_2(\mathcal{D}))$  for any  $p \in [1, \infty)$ —or, in other words, the probability distribution of  $Z$  in (4.1) defines a Gaussian measure on the Hilbert space  $L_2(\mathcal{D})$ —if and only if  $\beta \in (d/4, \infty)$ .*

In the case that the parameters in (4.1) and (4.2) are given by the triple

$$(\beta, \mathbf{a}, \kappa) \in \mathbb{R}_+ \times C^\infty(\overline{\mathcal{D}})^{d \times d} \times C^\infty(\overline{\mathcal{D}}),$$

we say that  $Z$  solves the SPDE (4.1) for  $(\beta, \mathbf{a}, \kappa)$ . By Proposition 4.2 the probability distribution of the zero-mean generalized Whittle–Matérn field  $Z: \mathcal{D} \times \Omega \rightarrow \mathbb{R}$  solving (4.1) for the parameter triple  $(\beta, \mathbf{a}, \kappa)$  defines a Gaussian measure  $\mu_d(0; \beta, \mathbf{a}, \kappa)$  on  $L_2(\mathcal{D})$  if and only if  $\beta \in (d/4, \infty)$ . In this case, for every Borel set  $B \in \mathcal{B}(L_2(\mathcal{D}))$ , it is given by

$$\mu_d(0; \beta, \mathbf{a}, \kappa)(B) = \mathbb{P}(\{\omega \in \Omega : Z(\cdot, \omega) \in B, Z \text{ solves (4.1)}\}).$$

Thus, it has mean zero and trace-class covariance operator  $C = L^{-2\beta} \in \mathcal{L}(L_2(\mathcal{D}))$ , cf. (2.1),

$$\begin{aligned} (C\psi, \psi')_{L_2(\mathcal{D})} &= \int_{L_2(\mathcal{D})} (\psi, \phi)_{L_2(\mathcal{D})} (\phi, \psi')_{L_2(\mathcal{D})} d\mu(\phi) \\ &= \int_{\Omega} (\psi, Z(\cdot, \omega))_{L_2(\mathcal{D})} (Z(\cdot, \omega), \psi')_{L_2(\mathcal{D})} d\mathbb{P}(\omega) = (L^{-2\beta}\psi, \psi')_{L_2(\mathcal{D})}. \end{aligned}$$

In summary, for  $\beta \in (d/4, \infty)$ , the Whittle–Matérn field  $Z: \mathcal{D} \times \Omega \rightarrow \mathbb{R}$  in (4.1) induces a Gaussian measure on  $L_2(\mathcal{D})$  given by  $\mu_d(0; \beta, \mathbf{a}, \kappa) = \mathbf{N}(0, L^{-2\beta})$ , see (2.1). More generally, we consider for an arbitrary mean value function  $m \in L_2(\mathcal{D})$ :

$$\mu_d(m; \beta, \mathbf{a}, \kappa) := \mathbf{N}(m, L^{-2\beta}). \tag{4.5}$$

The goal of this section is to identify the following:

- (a) the Cameron–Martin space for the Gaussian measure  $\mu_d(m; \beta, \mathbf{a}, \kappa)$ , as well as necessary and sufficient conditions for the Cameron–Martin spaces of two measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  to be isomorphic and norm equivalent;
- (b) necessary and sufficient conditions for two measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  to be equivalent (respectively, orthogonal); and
- (c) necessary and sufficient conditions for  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  to provide uniformly asymptotically optimal linear prediction in the case that  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  is the correct model.

These questions are addressed in Subsections 4.2, 4.3 and 4.4. We will see that the necessary and sufficient conditions mentioned in (a), (b) and (c) above all include the requirement that  $\beta = \tilde{\beta}$ .

**Table 1.** Necessary and sufficient conditions for (a) isomorphic, norm equivalent Cameron–Martin spaces of the measures  $\mu := \mu_d(0; \beta, \mathbf{a}, \kappa)$  and  $\tilde{\mu} := \mu_d(0; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , (b) equivalence of measures  $\mu \sim \tilde{\mu}$ , and (c) uniformly asymptotically optimal linear prediction when misspecifying  $\mu$  by  $\tilde{\mu}$ . Here,  $\delta_{\mathbf{a}}(s) := \tilde{\mathbf{a}}(s) - \mathbf{a}(s)$ ,  $\delta_{c, \kappa^2}(s) := \tilde{\kappa}^2(s) - c\kappa^2(s)$ ,  $\delta_{\kappa^2}(s) := \delta_{1, \kappa^2}(s)$ ,  $\mathbf{n}$  is the outward pointing normal on  $\partial\mathcal{D}$ , and “b.c.” stands for “boundary conditions”.

Conditions for	Interval for $\beta$ , assuming that $\beta \notin \{k + 1/4 : k \in \mathbb{N}\}$			
	$(d/4, 5/4)$	$(5/4, 9/4)$	$(9/4, 13/4)$	$(13/4, \infty)$
Isomorphic Cameron–Martin spaces	$\beta = \tilde{\beta}$	$\beta = \tilde{\beta}$ + b.c. on $\delta_{\mathbf{a}}$	$\beta = \tilde{\beta}$ + b.c. on $\delta_{\mathbf{a}}$ and $\delta_{\kappa^2}$	
Asymptotically optimal linear prediction	$\beta = \tilde{\beta}, c\mathbf{a} = \tilde{\mathbf{a}}$ for some $c \in (0, \infty)$		$\beta = \tilde{\beta}, c\mathbf{a} = \tilde{\mathbf{a}},$ $(\mathbf{a}\nabla\delta_{c, \kappa^2}) _{\partial\mathcal{D}} \cdot \mathbf{n} = 0$	$\beta = \tilde{\beta}, c\mathbf{a} = \tilde{\mathbf{a}}$ + b.c. on $\delta_{c, \kappa^2}$
Equivalence of measures in dimension $d \leq 3$	$\beta = \tilde{\beta}, \mathbf{a} = \tilde{\mathbf{a}}$		$\beta = \tilde{\beta}, \mathbf{a} = \tilde{\mathbf{a}},$ $(\mathbf{a}\nabla\delta_{\kappa^2}) _{\partial\mathcal{D}} \cdot \mathbf{n} = 0$	$\beta = \tilde{\beta}, \mathbf{a} = \tilde{\mathbf{a}}$ + b.c. on $\delta_{\kappa^2}$
Equivalence of measures in dimension $d \geq 4$	$\beta = \tilde{\beta}, \mathbf{a} = \tilde{\mathbf{a}}, \kappa^2 = \tilde{\kappa}^2$			

Depending on the value of  $\beta \in (d/4, \infty)$ , it is solely the behavior of  $\delta_{\mathbf{a}} := \tilde{\mathbf{a}} - \mathbf{a}$  and  $\delta_{\kappa^2} := \tilde{\kappa}^2 - \kappa^2$  at the boundary  $\partial\mathcal{D}$  that matters for (a), see Theorem 4.7. Finally, for (b) and (c) also conditions on  $\mathbf{a}, \tilde{\mathbf{a}}$  and  $\kappa^2, \tilde{\kappa}^2$  inside the domain  $\mathcal{D} \subset \mathbb{R}^d$  are imposed which for (b), equivalence of measures, additionally depend on the dimension  $d \in \mathbb{N}$ , see Theorems 4.11 and 4.13. We summarize the main outcomes of these theorems in Table 1.

### 4.2. Cameron–Martin spaces

We first characterize the function spaces which in the context of Whittle–Matérn fields act as Cameron–Martin spaces. The next result is a generalization of [31, Lemma 3.1] (where  $L = -\Delta$  and  $r \in \mathbb{N}_0$ ).

**Lemma 4.3.** *Suppose that Assumptions 4.1.I–III are satisfied and let  $\dot{H}_L^r$  be defined according to (2.3) with  $E = L_2(\mathcal{D})$  and  $L$  as in (4.2). Then, for every  $r \in \mathbb{R}_+$ , the space  $\dot{H}_L^r$  is a subspace of  $H^r(\mathcal{D})$  and  $(\dot{H}_L^r, \|\cdot\|_{r, L}) \hookrightarrow (H^r(\mathcal{D}), \|\cdot\|_{H^r(\mathcal{D})})$ . Furthermore, for every  $r \in \mathbb{R}_+ \setminus \mathfrak{E}$ , where*

$$\mathfrak{E} := \{2k + 1/2 : k \in \mathbb{N}_0\}, \tag{4.6}$$

*we have the identification*

$$\dot{H}_L^r = \{v \in H^r(\mathcal{D}) : (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j v = 0 \text{ in } L_2(\partial\mathcal{D}) \ \forall j \in \mathbb{N}_0 \text{ with } j \leq \lfloor \frac{2r-1}{4} \rfloor\}, \tag{4.7}$$

*and on the space  $\dot{H}_L^r$  the norm  $\|\cdot\|_{r, L}$  is equivalent to the Sobolev norm  $\|\cdot\|_{H^r(\mathcal{D})}$ .*

**Remark 4.4.** The coefficients  $\mathbf{a}, \kappa$  of the second-order differential operator  $L$  in (4.2) enter the characterization (4.7) of the Hilbert space  $\dot{H}_L^r$  (that is, the domain of the operator  $L^{r/2}$ ) only for  $r > 5/2$ . In this case, it is solely the behavior of  $\mathbf{a}$  and  $\kappa$  at the boundary  $\partial\mathcal{D}$  that determines  $\dot{H}_L^r$ . If  $r \in \mathfrak{E}$  belongs to the exception set, then the norm  $\|\cdot\|_{r, L}$  generates a strictly finer topology than the Sobolev norm  $\|\cdot\|_{H^r(\mathcal{D})}$ , cf. [24, Theorem 11.7 in Chapter 1]. We discuss this further in Section 6.

**Proof of Lemma 4.3.** We recall that by the divergence theorem, Theorem A.5 in Appendix A, we have

$$\begin{aligned} & (v_1, (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))v_2)_{L_2(\mathcal{D})} - ((\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))v_1, v_2)_{L_2(\mathcal{D})} \\ &= \int_{\partial\mathcal{D}} [v_2(\mathbf{a}\nabla v_1 \cdot \mathbf{n}) - v_1(\mathbf{a}\nabla v_2 \cdot \mathbf{n})] \, dS \quad \forall v_1, v_2 \in H^2(\mathcal{D}), \end{aligned} \tag{4.8}$$

where  $dS$  is the  $(d - 1)$ -dimensional surface measure on  $\partial\mathcal{D}$  and  $\mathbf{n}: \partial\mathcal{D} \rightarrow \mathbb{R}^d$  is the outward pointing unit normal vector field, see also Subsection A.1.2 and Remark A.2 in Appendix A.

**Step 1:**  $\supseteq$  in (4.7). First, we consider the case  $r \in (0, 2]$ ,  $r \neq 1/2$ , in (4.7). The equivalence

$$(\dot{H}_L^r, \|\cdot\|_{r,L}) \cong (H^r(\mathcal{D}) \cap H_0^1(\mathcal{D}), \|\cdot\|_{H^r(\mathcal{D})}), \quad r \in [1, 2], \tag{4.9}$$

can be shown in a similar manner as [12, Lemma 2]. Moreover, since  $\dot{H}_L^0 = L_2(\mathcal{D})$  and  $\dot{H}_L^1 = H_0^1(\mathcal{D})$ , it follows from [17, Theorem 8.1] that

$$(\dot{H}_L^r, \|\cdot\|_{r,L}) \cong (\{v \in H^r(\mathcal{D}) : v = 0 \text{ in } L_2(\partial\mathcal{D})\}, \|\cdot\|_{H^r(\mathcal{D})}), \quad r \in (1/2, 1), \tag{4.10}$$

$$(\dot{H}_L^r, \|\cdot\|_{r,L}) \cong (H^r(\mathcal{D}), \|\cdot\|_{H^r(\mathcal{D})}), \quad r \in (0, 1/2), \tag{4.11}$$

see also [24, Theorems 11.5 and 11.6 in Chapter 1].

Now let  $r = 2k + r_0$  for some  $k \in \mathbb{N}$  and  $r_0 \in (0, 1/2)$ , and assume in addition that  $v \in H^r(\mathcal{D})$  is such that  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j v = 0$  in  $L_2(\partial\mathcal{D})$  for all  $j \in \{0, 1, \dots, k - 1\}$ . Then, by using the boundary conditions of  $v$  and of the eigenfunctions  $\{e_j\}_{j \in \mathbb{N}}$  in (4.8), we obtain that

$$\begin{aligned} \|v\|_{r,L}^2 &= \sum_{j \in \mathbb{N}} \lambda_j^{2k+r_0} (v, e_j)_{L_2(\mathcal{D})}^2 = \sum_{j \in \mathbb{N}} \lambda_j^{r_0} (v, (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k e_j)_{L_2(\mathcal{D})}^2 \\ &= \sum_{j \in \mathbb{N}} \lambda_j^{r_0} ((\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v, e_j)_{L_2(\mathcal{D})}^2 = \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v\|_{r_0,L}^2. \end{aligned} \tag{4.12}$$

By the identification (4.11), there exist constants  $C', C \in \mathbb{R}_+$ , independent of  $v$ , such that

$$\|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v\|_{r_0,L}^2 \leq C' \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v\|_{H^{r_0}(\mathcal{D})}^2 \leq C \|v\|_{H^{2k+r_0}(\mathcal{D})}^2, \tag{4.13}$$

where we used the regularity of  $\kappa \in C^\infty(\overline{\mathcal{D}})$ ,  $\mathbf{a} \in C^\infty(\overline{\mathcal{D}})^{d \times d}$  in the last step. This shows that  $v \in \dot{H}_L^r$  and  $\|v\|_{r,L} \leq C \|v\|_{H^r(\mathcal{D})}$ , where the constant  $C \in \mathbb{R}_+$  is independent of  $v$ .

Assume now that  $r = 2k + r_0$  for some  $k \in \mathbb{N}$  and  $r_0 \in (1/2, 2]$ , and let  $v \in H^r(\mathcal{D})$  be such that  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j v = 0$  in  $L_2(\partial\mathcal{D})$  for all  $j \in \{0, 1, \dots, k\}$ . Then, as in (4.12), we obtain that  $\|v\|_{r,L}^2 = \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v\|_{r_0,L}^2$ . Since by assumption also the trace of  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^k v$  vanishes in  $L_2(\partial\mathcal{D})$ , we conclude by the equivalences in (4.9) and (4.10) that the estimates in (4.13) also hold in this case, with  $C', C \in \mathbb{R}_+$  independent of  $v$ .

**Step 2:**  $\subseteq$  in (4.7). For the reverse inclusion we show that **a**) for all  $r \in \mathbb{R}_+$  and all  $v \in \dot{H}_L^r$ , we have that  $v \in H^r(\mathcal{D})$  with  $\|v\|_{H^r(\mathcal{D})} \leq C \|v\|_{r,L}$ , and **b**) in the case that  $r \notin \mathfrak{E}$ , see (4.6), every  $v \in \dot{H}_L^r$  also satisfies the boundary conditions in (4.7). For **a**) we first prove the regularity result  $(\dot{H}_L^r, \|\cdot\|_{r,L}) \hookrightarrow (H^r(\mathcal{D}), \|\cdot\|_{H^r(\mathcal{D})})$  for all integers  $r \in \{2k - 1, 2k\} : k \in \mathbb{N}\}$ , via induction with respect to  $k \in \mathbb{N}$ . The cases  $r \in \{1, 2\}$  (i.e.,  $k = 1$ ) are part of (4.9).

For the induction step  $k - 1 \rightarrow k$ , let  $k \geq 2$  and  $v \in \dot{H}_L^{2k-1} = \mathcal{D}(L^{k-1/2})$ . Then, there exists  $\psi \in L_2(\mathcal{D})$  such that  $v = L^{-(k-1/2)}\psi$  and  $\tilde{v} := L^{-(k-3/2)}\psi$  satisfies  $\tilde{v} \in \mathcal{D}(L^{k-3/2}) = \dot{H}_L^{2k-3}$ . Thus,  $Lv = \tilde{v} \in H^{2k-3}(\mathcal{D})$  follows from the induction hypothesis, and there exists a constant  $C' \in \mathbb{R}_+$ , which is independent of

$v \in \dot{H}_L^{2k-1}$ , such that  $\|Lv\|_{H^{2k-3}(\mathcal{D})} \leq C'\|Lv\|_{2k-3,L} = C'\|v\|_{2k-1,L}$ . As  $v \in \dot{H}_L^{2k-1} \subset \mathcal{D}(L)$ , this regularity of  $Lv \in H^{2k-3}(\mathcal{D})$  implies by Theorem A.6 that  $v \in H^{2k-1}(\mathcal{D})$ ,

$$\begin{aligned} \|v\|_{H^{2k-1}(\mathcal{D})} &\leq \widehat{C} (\|Lv\|_{H^{2k-3}(\mathcal{D})} + \|v\|_{H^{2k-2}(\mathcal{D})}) \\ &\leq \widehat{C} (C'\|v\|_{2k-1,L} + C''\|v\|_{2k-2,L}) \leq C\|v\|_{2k-1,L}, \end{aligned}$$

where all constants are independent of  $v$ . In this step, we also used that by the induction hypothesis  $(\dot{H}_L^{2k-2}, \|\cdot\|_{2k-2,L}) \hookrightarrow (H^{2k-2}(\mathcal{D}), \|\cdot\|_{H^{2k-2}(\mathcal{D})})$  holds. Suppose now that  $v \in \dot{H}_L^{2k} = \mathcal{D}(L^k)$ . Then, similarly as above, we obtain from the induction hypothesis that  $Lv \in H^{2k-2}(\mathcal{D})$  with norm bounded by  $\|Lv\|_{H^{2k-2}(\mathcal{D})} \leq C'\|v\|_{2k,L}$  and, again by Theorem A.6, the regularity  $v \in H^{2k}(\mathcal{D})$  follows, with

$$\|v\|_{H^{2k}(\mathcal{D})} \leq \widehat{C} (\|Lv\|_{H^{2k-2}(\mathcal{D})} + \|v\|_{H^{2k-1}(\mathcal{D})}) \leq C\|v\|_{2k,L}.$$

By means of complexification and interpolation arguments (see Lemma F.3 in the Supplementary Material [6], [32, Theorem 1 in Section 4.3.1] and [25, Theorem 2.6]) we subsequently obtain the continuous embedding  $(\dot{H}_L^r, \|\cdot\|_{r,L}) \hookrightarrow (H^r(\mathcal{D}), \|\cdot\|_{H^r(\mathcal{D})})$  for the whole range  $r \in \mathbb{R}_+$ .

**Step 2b)** Finally, it can also be shown via induction with respect to  $k \in \mathbb{N}_0$  that

$$\begin{aligned} \forall r \in (2k, 2k + 1/2), \quad \forall v \in \dot{H}_L^r : \quad &(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j v = 0 \text{ in } L_2(\partial\mathcal{D}), \quad 0 \leq j \leq k - 1, \\ \forall r \in (2k + 1/2, 2k + 2], \quad \forall v \in \dot{H}_L^r : \quad &(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j v = 0 \text{ in } L_2(\partial\mathcal{D}), \quad 0 \leq j \leq k. \end{aligned}$$

Specifically, the case  $k = 0$  is part of (4.9), (4.10) and (4.11). For the induction step  $k - 1 \rightarrow k$ , let  $k \in \mathbb{N}$ , and  $v_1 \in \dot{H}_L^{r_1}$ ,  $v_2 \in \dot{H}_L^{r_2}$ , where  $r_1 \in (2k, 2k + 1/2)$  and  $r_2 \in (2k + 1/2, 2k + 2]$ . As we have already proven, Sobolev regularity follows:  $v_1 \in H^{r_1}(\mathcal{D})$  and  $v_2 \in H^{r_2}(\mathcal{D})$ . Since  $r_1 > 2k$  and  $r_2 > 2k + 1/2$ , the trace theorem, Theorem A.3 in Appendix A, guarantees that the traces are well-defined,  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_1} v_1 \in L_2(\partial\mathcal{D})$  and  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_2} v_2 \in L_2(\partial\mathcal{D})$  for all  $j_1 \in \{0, 1, \dots, k - 1\}$  and  $j_2 \in \{0, 1, \dots, k\}$ , respectively. Furthermore, the induction hypothesis implies that  $Lv_1 \in \dot{H}_L^{r_1-2}$  and  $Lv_2 \in \dot{H}_L^{r_2-2}$  satisfy the boundary conditions

$$\begin{aligned} (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_1} v_1 &= (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_1-1} (Lv_1) = 0 \text{ in } L_2(\partial\mathcal{D}), \quad 1 \leq j_1 \leq k - 1, \\ (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_2} v_2 &= (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^{j_2-1} (Lv_2) = 0 \text{ in } L_2(\partial\mathcal{D}), \quad 1 \leq j_2 \leq k. \end{aligned}$$

Since  $v_1, v_2 \in \dot{H}_L^2 = H^2(\mathcal{D}) \cap H_0^1(\mathcal{D})$ , we obtain that also  $v_1 = v_2 = 0$  in  $L_2(\partial\mathcal{D})$ . □

Now we are ready to characterize the Cameron–Martin space for  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  in (4.5).

**Proposition 4.5.** *Let  $d \in \mathbb{N}$ ,  $\beta \in (d/4, \infty)$ ,  $m \in L_2(\mathcal{D})$  and suppose Assumptions 4.1.I–III. Then, the Cameron–Martin space of the Gaussian measure  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  in (4.5) with covariance operator  $C = L^{-2\beta}$  is given by  $C^{1/2}(L_2(\mathcal{D})) = \dot{H}_L^{2\beta}$ , cf. (2.3), and it is continuously embedded in  $H^{2\beta}(\mathcal{D})$ .*

*In the case that  $2\beta \notin \mathfrak{E}$ , with  $\mathfrak{E}$  as given in (4.6), it can be identified as in (4.7) and there exist constants  $c_0, c_1, c_0^*, c_1^* > 0$ , depending on  $\beta, \mathbf{a}, \kappa, \mathcal{D}$ , such that*

$$c_0 \|v\|_{H^{2\beta}(\mathcal{D})}^2 \leq (C^{-1/2}v, C^{-1/2}v)_{L_2(\mathcal{D})} \leq c_1 \|v\|_{H^{2\beta}(\mathcal{D})}^2 \quad \forall v \in \dot{H}_L^{2\beta} = C^{1/2}(L_2(\mathcal{D})), \quad (4.14)$$

$$c_0^* \|v\|_{H^{-2\beta}(\mathcal{D})}^2 \leq (C^{1/2}v, C^{1/2}v)_{L_2(\mathcal{D})} \leq c_1^* \|v\|_{H^{-2\beta}(\mathcal{D})}^2 \quad \forall v \in \dot{H}_L^{-2\beta} = C^{-1/2}(L_2(\mathcal{D})). \quad (4.15)$$

**Proof.** That the Cameron–Martin space is given by  $\dot{H}_L^{2\beta}$  has already been observed in (2.4). Furthermore, whenever  $2\beta \notin \mathfrak{E} = \{2k + 1/2 : k \in \mathbb{N}_0\}$ , we obtain (4.14) from Lemma 4.3 which also implies the norm equivalence (4.15) on  $\dot{H}_L^{-2\beta}$  as this is the dual space of  $\dot{H}_L^{2\beta}$ .  $\square$

**Remark 4.6.** Proposition 4.5 shows that under Assumptions 4.1.I–III the Cameron–Martin space for the Gaussian measure  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  in (4.5) with  $\beta \in (d/4, \infty)$  is

$$C^{1/2}(L_2(\mathcal{D})) = \dot{H}_L^{2\beta} \hookrightarrow H^{2\beta}(\mathcal{D}) \hookrightarrow C^0(\overline{\mathcal{D}}),$$

where the last relation is one of the Sobolev embeddings, see e.g. [32, Theorem 4.6.1.(e)]. In particular, the random field  $Z : \overline{\mathcal{D}} \times \Omega \rightarrow \mathbb{R}$  which solves the SPDE (4.1) for  $(\beta, \mathbf{a}, \kappa)$  is continuous ( $\mathbb{P}$ -almost surely and in  $L_p$ -sense for any  $p \in [1, \infty)$ ) and its covariance kernel  $\varrho$  is continuous on  $\overline{\mathcal{D}} \times \overline{\mathcal{D}}$ .

An important consequence of Proposition 4.5 and Lemma 2.2(iii) is the following result on equivalence of Cameron–Martin spaces for Gaussian measures defined as in (4.5) with different parameters.

**Theorem 4.7.** *Suppose Assumption 4.1.III and that each of the parameter tuples  $(\mathbf{a}, \kappa)$ ,  $(\tilde{\mathbf{a}}, \tilde{\kappa})$  fulfills Assumptions 4.1.I–II. Let  $\beta \in \mathbb{R}_+$  be such that  $2\beta \notin \mathfrak{E}$ , with  $\mathfrak{E}$  as in (4.6), and let  $L, \tilde{L}$  be defined as in (4.2) with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively. Then, for all  $\gamma \in [-\beta, \beta]$ , the operator  $\tilde{L}^\gamma L^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  (and, thus,  $\dot{H}_L^{2\gamma}, \dot{H}_{\tilde{L}}^{2\gamma}$  are norm equivalent spaces) if and only if, for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ , the following hold:*

$$\begin{aligned} \forall v \in \dot{H}_L^{2\beta} : \quad & (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2} - \nabla \cdot (\delta_{\mathbf{a}}\nabla))v = 0 \text{ in } L_2(\partial\mathcal{D}), \\ \forall \tilde{v} \in \dot{H}_{\tilde{L}}^{2\beta} : \quad & (\tilde{\kappa}^2 - \nabla \cdot (\tilde{\mathbf{a}}\nabla))^j (\delta_{\tilde{\kappa}^2} - \nabla \cdot (\delta_{\tilde{\mathbf{a}}}\nabla))\tilde{v} = 0 \text{ in } L_2(\partial\mathcal{D}). \end{aligned} \tag{4.16}$$

Here, we set  $\delta_{\kappa^2}(s) := \tilde{\kappa}^2(s) - \kappa^2(s)$  and  $\delta_{\mathbf{a}}(s) := \tilde{\mathbf{a}}(s) - \mathbf{a}(s)$  for all  $s \in \overline{\mathcal{D}}$ .

Furthermore, the Cameron–Martin spaces of two Gaussian measures  $\mu_d(0; \beta, \mathbf{a}, \kappa)$ ,  $\mu_d(0; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , defined according to (4.5) with  $\beta, \tilde{\beta} \in (d/4, \infty)$ , where  $d \in \mathbb{N}$  and  $2\beta \notin \mathfrak{E}$ , are isomorphic with equivalent norms if and only if  $\beta = \tilde{\beta}$  and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ .

**Proof.** In order to derive the first assertion, we distinguish two cases, **Case I:**  $\beta \in (0, 1)$ ,  $\beta \neq 1/4$  and **Case II:**  $\beta \in [1, \infty)$ ,  $2\beta \notin \mathfrak{E}$ .

In **Case I**,  $\beta \in (0, 1)$ ,  $\beta \neq 1/4$ , there are no conditions imposed in (4.16) and we obtain the relation  $(\dot{H}_L^{2\beta}, \|\cdot\|_{2\beta, L}) \cong (\dot{H}_{\tilde{L}}^{2\beta}, \|\cdot\|_{2\beta, \tilde{L}})$  from one of the identifications in (4.9), (4.10) or (4.11). Consequently,  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and by complexification and interpolation, see Lemma F.3 in Appendix F, the same is true for  $\tilde{L}^\gamma L^{-\gamma}$  and all  $\gamma \in [-\beta, \beta]$ .

**Case II:** For  $\beta \in [1, \infty)$ , Lemma 2.2(iii) shows that  $\tilde{L}^\gamma L^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  for every  $\gamma \in [-\beta, \beta]$  if and only if  $\tilde{L} - L \in \mathcal{L}(\dot{H}_L^{2\eta}; \dot{H}_L^{2(\eta-1)}) \cap \mathcal{L}(\dot{H}_{\tilde{L}}^{2\eta}; \dot{H}_{\tilde{L}}^{2(\eta-1)})$  holds for  $\eta \in \{1, \beta\}$ . The claim then follows from identifying  $\dot{H}_L^{2\beta-2}$  and  $\dot{H}_{\tilde{L}}^{2\beta-2}$  according to (4.7) in Lemma 4.3, combined with the regularity  $(\tilde{L} - L)v \in H^{2\eta-2}(\mathcal{D})$  which holds for all  $v \in \dot{H}_L^{2\eta} \cup \dot{H}_{\tilde{L}}^{2\eta} \subseteq H^{2\eta}(\mathcal{D})$  and every  $\eta \in \{1, \beta\}$ , since  $\kappa, \tilde{\kappa} \in C^\infty(\overline{\mathcal{D}})$  and  $\mathbf{a}, \tilde{\mathbf{a}} \in C^\infty(\overline{\mathcal{D}})^{d \times d}$  are smooth.

We now prove the second claim. By Proposition 4.5 the Cameron–Martin spaces are  $\dot{H}_L^{2\beta}$  and  $\dot{H}_{\tilde{L}}^{2\beta}$ . If we identify the Hilbert space  $L_2(\mathcal{D})$  with the space  $\ell^2$  of square-summable sequences, Weyl’s law (4.4) (applied for  $L$  and  $\tilde{L}$ ) shows that  $\dot{H}_L^{2\beta}$  can be identified with  $\{(c_j)_{j \in \mathbb{N}} : \{j^{2\beta/d} c_j\}_{j \in \mathbb{N}} \in \ell^2\} \subset \ell^2$  and



$\dot{H}_L^{2\tilde{\beta}}$  with  $\{(\tilde{c}_j)_{j \in \mathbb{N}} : \{j^{2\tilde{\beta}/d} \tilde{c}_j\}_{j \in \mathbb{N}} \in \ell^2\} \subset \ell^2$ . For this reason,  $\dot{H}_L^{2\beta}$  and  $\dot{H}_L^{2\tilde{\beta}}$  can be isomorphic only if  $\beta = \tilde{\beta}$ . In the case that  $\beta = \tilde{\beta}$  and  $2\beta \notin \mathfrak{E}$ , sufficiency and necessity of the conditions (4.16) for  $\dot{H}_L^{2\beta}$  and  $\dot{H}_L^{2\tilde{\beta}} = \dot{H}_L^{2\beta}$  to be isomorphic follow from the first part of this theorem.  $\square$

We end this subsection with a discussion of the conditions (4.16). In what follows, we suppose that the assumptions of Theorem 4.7 on the coefficients of  $L, \tilde{L}$  and on the domain  $\mathcal{D} \subset \mathbb{R}^d$  are satisfied. Firstly, we note that for  $\beta \in (0, 5/4)$  no boundary conditions on  $\delta_{\kappa^2}$  or  $\delta_{\mathbf{a}}$  are imposed and the spaces  $\dot{H}_L^{2\beta}$  and  $\dot{H}_L^{2\tilde{\beta}}$  are isomorphic, independently of the choice of  $\kappa, \tilde{\kappa}, \mathbf{a}, \tilde{\mathbf{a}}$ . Next, consider the case that  $\beta \in (5/4, 9/4)$ . Then, the conditions (4.16) say that

$$(\delta_{\kappa^2} - \nabla \cdot (\delta_{\mathbf{a}} \nabla))v = (\tilde{\kappa}^2 - \nabla \cdot (\tilde{\mathbf{a}} \nabla))v - (\kappa^2 - \nabla \cdot (\mathbf{a} \nabla))v = 0 \text{ in } L_2(\partial \mathcal{D})$$

has to hold for every  $v \in \dot{H}_L^{2\beta} \cup \dot{H}_L^{2\tilde{\beta}}$ . By (4.7), for all  $\beta \in (5/4, \infty)$ , every  $v \in \dot{H}_L^{2\beta} \cup \dot{H}_L^{2\tilde{\beta}}$  satisfies the boundary condition  $v = 0$  in  $L_2(\partial \mathcal{D})$ . Therefore, in this case (4.16) simplifies to the requirement that  $\nabla \cdot (\delta_{\mathbf{a}} \nabla v) = 0$  in  $L_2(\partial \mathcal{D})$  for all  $v \in \dot{H}_L^{2\beta} \cup \dot{H}_L^{2\tilde{\beta}}$ . In particular, note that no assumptions are imposed on  $\kappa, \tilde{\kappa}$ . Finally, we consider the case that  $c\mathbf{a} = \tilde{\mathbf{a}}$  for some  $c \in \mathbb{R}_+$  and  $\beta \in (9/4, 13/4)$ . Since  $\dot{H}_L^{2\beta} \cong \dot{H}_L^{2\tilde{\beta}}$  holds if and only if  $\dot{H}_{cL}^{2\beta} \cong \dot{H}_L^{2\tilde{\beta}}$ , we thus need that for all  $v \in \dot{H}_L^{2\beta} = \dot{H}_{cL}^{2\beta}$  and  $\tilde{v} \in \dot{H}_L^{2\tilde{\beta}}$ :

$$(\kappa^2 - \nabla \cdot (\mathbf{a} \nabla))(\delta_{c, \kappa^2} v) = 0 \text{ in } L_2(\partial \mathcal{D}) \quad \text{and} \quad (\tilde{\kappa}^2 - c \nabla \cdot (\mathbf{a} \nabla))(\delta_{c, \kappa^2} \tilde{v}) = 0 \text{ in } L_2(\partial \mathcal{D}), \quad (4.17)$$

where  $\delta_{c, \kappa^2}(s) := \tilde{\kappa}^2(s) - c\kappa^2(s)$ . Since  $(\kappa^2 - \nabla \cdot (\mathbf{a} \nabla))v = v = 0$  in  $L_2(\partial \mathcal{D})$ , this gives

$$\begin{aligned} 0 &= (\kappa^2 - \nabla \cdot (\mathbf{a} \nabla))(\delta_{c, \kappa^2} v) = \delta_{c, \kappa^2}(\kappa^2 - \nabla \cdot (\mathbf{a} \nabla))v - 2(\mathbf{a} \nabla v) \cdot \nabla \delta_{c, \kappa^2} - v \nabla \cdot (\mathbf{a} \nabla \delta_{c, \kappa^2}) \\ &= -2(\mathbf{a} \nabla v) \cdot \nabla \delta_{c, \kappa^2} \text{ in } L_2(\partial \mathcal{D}), \end{aligned}$$

for all  $v \in \dot{H}_L^{2\beta}$  and, similarly,  $(\mathbf{a} \nabla \tilde{v}) \cdot \nabla \delta_{c, \kappa^2} = 0$  in  $L_2(\partial \mathcal{D})$  follows for all  $\tilde{v} \in \dot{H}_L^{2\tilde{\beta}}$ . The traces of  $v, \tilde{v}$  vanish in  $L_2(\partial \mathcal{D})$  and  $\partial \mathcal{D}$  is smooth. Therefore, also the traces of all tangential components of  $\nabla v, \nabla \tilde{v}$  vanish and  $\nabla v = \frac{\partial v}{\partial \mathbf{n}} \mathbf{n}$ ,  $\nabla \tilde{v} = \frac{\partial \tilde{v}}{\partial \mathbf{n}} \mathbf{n}$  with equality in  $L_2(\partial \mathcal{D}; \mathbb{R}^d)$ , where  $\mathbf{n}$  is the outward pointing unit normal on  $\partial \mathcal{D}$ , see Remark A.2 in Appendix A. For  $\beta \in (9/4, 13/4)$  and  $r \in (3/2, 2)$ ,  $\dot{H}_L^{2\beta}, \dot{H}_L^{2\tilde{\beta}}$  are dense in  $H^r(\mathcal{D}) \cap H_0^1(\mathcal{D})$  and the trace map  $v \mapsto \{\frac{\partial^j v}{\partial \mathbf{n}^j} : j = 0, 1\}$  of  $H^r(\mathcal{D}) \rightarrow H^{r-1/2}(\partial \mathcal{D}) \times H^{r-3/2}(\partial \mathcal{D})$  is surjective, see Theorem A.3 in Appendix A. Since also  $H^{r-3/2}(\partial \mathcal{D})$  is dense in  $L_2(\partial \mathcal{D})$ , the requirement (4.17) simplifies to the following condition on  $\delta_{c, \kappa^2} = \tilde{\kappa}^2 - c\kappa^2$ :

$$\begin{aligned} \forall v \in \dot{H}_L^{2\beta} : \quad & (\mathbf{a} \nabla v) \cdot \nabla \delta_{c, \kappa^2} = \frac{\partial v}{\partial \mathbf{n}}(\mathbf{a} \mathbf{n}) \cdot \nabla \delta_{c, \kappa^2} = 0 \text{ in } L_2(\partial \mathcal{D}) \\ \iff & (\mathbf{a} \nabla \delta_{c, \kappa^2}) \cdot \mathbf{n} = 0 \text{ on } \partial \mathcal{D}. \end{aligned} \quad (4.18)$$

### 4.3. Equivalence and orthogonality of Whittle–Matérn measures

The main outcomes of this section are necessary and sufficient conditions on the parameters involved for two Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , defined according to (4.5), to be equivalent, see Theorem 4.11. In order to derive this result, we first formulate three lemmas which will guarantee sufficiency (Lemma 4.8) and necessity (Lemmas 4.9 and 4.10) of the conditions.

**Lemma 4.8.** *Let  $d \in \{1, 2, 3\}$  and let  $\beta \in (d/4, \infty)$  be such that  $2\beta \notin \mathfrak{E}$ , with  $\mathfrak{E}$  as given in (4.6). In addition, suppose Assumption 4.1.III and let the operators  $L$  and  $\tilde{L}$  be defined as in (4.2) with coefficients  $\mathbf{a}, \kappa$  and  $\mathbf{a}, \tilde{\kappa}$ , respectively, where  $\mathbf{a}$  fulfills Assumption 4.1.I and  $\kappa, \tilde{\kappa}$  are such that Assumption 4.1.II is satisfied and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ . Then, the operator  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$  is Hilbert–Schmidt on  $L_2(\mathcal{D})$ .*

**Proof.** Firstly, we note that by Theorem 4.7 the operator  $\tilde{L}^\gamma L^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  for all  $\gamma \in [-\beta, \beta]$ . To prove the Hilbert–Schmidt property of  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$ , we distinguish between

**Case I:**  $\beta \in (d/4, 1)$  and **Case II:**  $\beta \in [1, \infty)$ ,  $2\beta \notin \mathfrak{E}$ .

**Case I:** For  $\beta \in (d/4, 1)$ , we first observe the identity

$$\begin{aligned} \tilde{L}^{2\beta} - L^{2\beta} &= \frac{1}{2}(\tilde{L}^\beta + L^\beta)(\tilde{L}^\beta - L^\beta) + \frac{1}{2}(\tilde{L}^\beta - L^\beta)(\tilde{L}^\beta + L^\beta) \\ &= \frac{1}{2}(\tilde{L}^\beta + L^\beta)(\tilde{L}^\beta - L^\beta) + \frac{1}{2}[(\tilde{L}^\beta + L^\beta)(\tilde{L}^\beta - L^\beta)]^*. \end{aligned}$$

Since for  $S \in \mathcal{L}_2(E)$  we have  $S^* \in \mathcal{L}_2(E)$  with  $\|S^*\|_{\mathcal{L}_2(E)} = \|S\|_{\mathcal{L}_2(E)}$ , we estimate

$$\begin{aligned} \|L^{-\beta}(\tilde{L}^{2\beta} - L^{2\beta})L^{-\beta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} &\leq \|L^{-\beta}(\tilde{L}^\beta + L^\beta)(\tilde{L}^\beta - L^\beta)L^{-\beta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} \\ &\leq (\|L^{-\beta}\tilde{L}^\beta\|_{\mathcal{L}(L_2(\mathcal{D}))} + 1)\|(\tilde{L}^\beta - L^\beta)L^{-\beta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))}. \end{aligned}$$

By the isomorphism property of  $\tilde{L}^\beta L^{-\beta}$ , the operator  $L^{-\beta}\tilde{L}^\beta$  is bounded on  $L_2(\mathcal{D})$ . Furthermore, since  $(\tilde{L} - L)\psi = \delta_{\kappa^2}\psi$  and  $\delta_{\kappa^2} := \tilde{\kappa}^2 - \kappa^2 \in C^\infty(\mathcal{D})$ , we find that  $\tilde{L} - L \in \mathcal{L}(L_2(\mathcal{D}))$ . Thus, by Lemma C.1 and Remark C.2 in the Supplementary Material [6], also  $\tilde{L}^\beta - L^\beta \in \mathcal{L}(L_2(\mathcal{D}))$ , and

$$\|(\tilde{L}^\beta - L^\beta)L^{-\beta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} \leq \|\tilde{L}^\beta - L^\beta\|_{\mathcal{L}(L_2(\mathcal{D}))} \|L^{-\beta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} < \infty.$$

Here, the Hilbert–Schmidt property of  $L^{-\beta} \in \mathcal{L}_2(L_2(\mathcal{D}))$  for  $\beta \in (d/4, 1)$  follows from the spectral asymptotics (4.4) of the operator  $L$  since, for any  $\varepsilon \in \mathbb{R}_+$ ,

$$\|L^{-(d/4+\varepsilon)}\|_{\mathcal{L}_2(L_2(\mathcal{D}))}^2 = \sum_{j \in \mathbb{N}} \lambda_j^{-d/2-2\varepsilon} \leq c_\lambda^{-d/2-2\varepsilon} \sum_{j \in \mathbb{N}} j^{-1-(4\varepsilon)/d} < \infty. \tag{4.19}$$

**Case II:** Let  $\mathfrak{R}_\beta$  be as in (2.5) and  $\eta \in \mathfrak{R}_\beta$ . Pick  $\varepsilon_0 \in (0, 1/2)$  such that  $2\eta - d/2 - \varepsilon_0 \notin \mathfrak{E}$  holds for all  $\eta \in \mathfrak{R}_\beta$ . Then, by Lemma 4.3, on  $\dot{H}_L^{2\eta-d/2-\varepsilon_0}$  the norm  $\|\cdot\|_{2\eta-d/2-\varepsilon_0, L}$  is equivalent to the Sobolev norm  $\|\cdot\|_{H^{2\eta-d/2-\varepsilon_0}(\mathcal{D})}$ . Furthermore,  $\dot{H}_L^{2\eta}$  is dense in  $\dot{H}_L^{2\eta-d/2-\varepsilon_0}$  and for any fixed  $\psi \in \dot{H}_L^{2\eta-d/2-\varepsilon_0}$ ,  $\delta \in \mathbb{R}_+$  there exists  $v_\delta \in \dot{H}_L^{2\eta}$  such that  $\|\psi - v_\delta\|_{2\eta-d/2-\varepsilon_0, L} < \delta$ . As (4.16) is assumed, for every  $\eta \in \mathfrak{R}_\beta$  and all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ , we have  $(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2} v) = 0$  in  $L_2(\partial\mathcal{D})$  for all  $v \in \dot{H}_L^{2\eta}$ . Since  $1 - \varepsilon_0 \in (1/2, 1)$ , by the trace theorem, Theorem A.3 in Appendix A, there are  $C, \widehat{C}, C' \in \mathbb{R}_+$  independent of  $\delta, v_\delta$  and  $\psi$  such that, for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ ,

$$\begin{aligned} \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2}\psi)\|_{L_2(\partial\mathcal{D})} &= \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2}(\psi - v_\delta))\|_{L_2(\partial\mathcal{D})} \\ &\leq C \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2}(\psi - v_\delta))\|_{H^{1-\varepsilon_0}(\mathcal{D})} \leq \widehat{C} \|\psi - v_\delta\|_{H^{2j+1-\varepsilon_0}(\mathcal{D})} \\ &\leq \widehat{C} \|\psi - v_\delta\|_{H^{2\eta-3/2-\varepsilon_0}(\mathcal{D})} \leq \widehat{C} \|\psi - v_\delta\|_{H^{2\eta-d/2-\varepsilon_0}(\mathcal{D})} \leq C' \|\psi - v_\delta\|_{2\eta-d/2-\varepsilon_0, L} < \delta. \end{aligned}$$

As  $\psi \in \dot{H}_L^{2\eta-d/2-\varepsilon_0}$  and  $\delta \in \mathbb{R}_+$  were arbitrary, we conclude that for every  $\eta \in \mathfrak{R}_\beta$  and all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ , the following behavior on the boundary is satisfied:

$$\forall \psi \in \dot{H}_L^{2\eta-d/2-\varepsilon_0} : (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{\kappa^2}\psi) = 0 \text{ in } L_2(\partial\mathcal{D}). \tag{4.20}$$

Furthermore, we have  $d/2 + \varepsilon_0 \in (1/2, 2)$ . Therefore, the regularity of  $\delta_{\kappa^2} \in C^\infty(\overline{\mathcal{D}})$  and (4.20) imply using the identification (4.7) for  $\dot{H}_L^{2(\eta-1)}$  that  $B := \tilde{L} - L \in \mathcal{L}(\dot{H}_L^{2\eta-d/2-\varepsilon_0}, \dot{H}_L^{2(\eta-1)})$  holds for every  $\eta \in \mathfrak{R}_\beta$ . This statement is equivalent to  $L^{\eta-1}BL^{-\eta+d/4+\varepsilon_0/2} \in \mathcal{L}(L_2(\mathcal{D}))$  and we conclude that the operator  $S_\eta := L^{\eta-1}\tilde{L}L^{-\eta} - \text{Id}_{L_2(\mathcal{D})} = L^{\eta-1}(\tilde{L} - L)L^{-\eta}$  is Hilbert–Schmidt on  $L_2(\mathcal{D})$ , since

$$\begin{aligned} \|L^{\eta-1}(\tilde{L} - L)L^{-\eta}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} &= \|L^{\eta-1}BL^{-\eta+d/4+\varepsilon_0/2}L^{-d/4-\varepsilon_0/2}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} \\ &\leq \|L^{\eta-1}BL^{-\eta+d/4+\varepsilon_0/2}\|_{\mathcal{L}(L_2(\mathcal{D}))}\|L^{-d/4-\varepsilon_0/2}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} < \infty \end{aligned}$$

follows for all  $\eta \in \mathfrak{R}_\beta$  by recalling (4.19). We thus obtain the Hilbert–Schmidt property of the operator  $L^{-\beta}\tilde{L}^{2\beta}L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$  from Lemma 2.2(i), using  $U_\eta = \text{Id}_{L_2(\mathcal{D})}$  for all  $\eta \in \mathfrak{R}_\beta$ .  $\square$

**Lemma 4.9.** *Let  $c \in \mathbb{R}_+$ ,  $d \in \mathbb{N}$ , and suppose Assumption 4.1.III. Let  $L$  and  $\tilde{L}$  be defined as in (4.2) with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively, where  $\mathbf{a}, \tilde{\mathbf{a}}$  fulfill Assumption 4.1.I and  $\kappa, \tilde{\kappa}$  satisfy Assumption 4.1.II. If  $c\mathbf{a} \neq \tilde{\mathbf{a}}$ , then the operator  $L^{-1/4}\tilde{L}^{1/2}L^{-1/4} - c^{1/2}\text{Id}_{L_2(\mathcal{D})}$  is not compact on  $L_2(\mathcal{D})$ .*

For ease of presentation, the proof is postponed to Appendix E in the Supplementary Material [6].

**Lemma 4.10.** *Let  $d \in \mathbb{N}$ ,  $d \geq 4$ , and suppose Assumption 4.1.III. Let the operators  $L$  and  $\tilde{L}$  be defined as in (4.2) with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively, where  $\mathbf{a}$  fulfills Assumption 4.1.I and  $\kappa, \tilde{\kappa}$  satisfy Assumption 4.1.II. If  $\kappa^2 \neq \tilde{\kappa}^2$ , then  $L^{-1/2}\tilde{L}L^{-1/2} - \text{Id}_{L_2(\mathcal{D})}$  is not Hilbert–Schmidt on  $L_2(\mathcal{D})$ .*

**Proof.** As in Theorem 4.7, we define  $\delta_{\kappa^2} \in C^\infty(\overline{\mathcal{D}})$  by  $\delta_{\kappa^2}(s) := \tilde{\kappa}^2(s) - \kappa^2(s)$ ,  $s \in \overline{\mathcal{D}}$ . Furthermore, we set  $\delta^+(s) := \max\{\delta_{\kappa^2}(s), 0\}$  and  $\delta^-(s) := -\min\{\delta_{\kappa^2}(s), 0\}$ ,  $s \in \overline{\mathcal{D}}$ .

**Step 1:** We first prove the claim for the case that either  $\delta^+(s) \geq \delta_0 \in \mathbb{R}_+$  holds for all  $s \in \overline{\mathcal{D}}$  or  $\delta^-(s) \geq \delta_0 \in \mathbb{R}_+$  holds for all  $s \in \overline{\mathcal{D}}$ . Then,  $\delta_{\kappa^2}^{-1}(s) := 1/\delta_{\kappa^2}(s)$  is well-defined,  $\delta_{\kappa^2}^{-1} \in C^\infty(\overline{\mathcal{D}})$ , and the multiplier  $M_{\delta_{\kappa^2}} : L_2(\mathcal{D}) \rightarrow L_2(\mathcal{D})$ ,  $v \mapsto \delta_{\kappa^2}v$ , is an isomorphism with  $M_{\delta_{\kappa^2}}^{-1} = M_{\delta_{\kappa^2}^{-1}}$ . Moreover, for every  $v \in H_0^1(\mathcal{D})$ , we have that  $\delta_{\kappa^2}v = \delta_{\kappa^2}^{-1}v = 0$  in  $L_2(\partial\mathcal{D})$  as well as  $\nabla(\delta_{\kappa^2}v) = v\nabla\delta_{\kappa^2} + \delta_{\kappa^2}\nabla v$  and  $\nabla(\delta_{\kappa^2}^{-1}v) = v\nabla\delta_{\kappa^2}^{-1} + \delta_{\kappa^2}^{-1}\nabla v$  in  $L_2(\mathcal{D})$ . Combining these observations with the identification  $(\dot{H}_L^1, \|\cdot\|_{1,L}) \cong (H_0^1(\mathcal{D}), \|\cdot\|_{H^1(\mathcal{D})})$ , see (4.7), shows that  $M_{\delta_{\kappa^2}}, M_{\delta_{\kappa^2}^{-1}} \in \mathcal{L}(\dot{H}_L^1)$ . Since the operators  $M_{\delta_{\kappa^2}}, M_{\delta_{\kappa^2}^{-1}}$  are self-adjoint on  $L_2(\mathcal{D})$ , also  $M_{\delta_{\kappa^2}}, M_{\delta_{\kappa^2}^{-1}} \in \mathcal{L}(\dot{H}_L^1)$  follows. We conclude that  $L^{-1/2}M_{\delta_{\kappa^2}}L^{1/2}$  is bounded on  $L_2(\mathcal{D})$  and has a bounded inverse,  $L^{-1/2}M_{\delta_{\kappa^2}^{-1}}L^{1/2} \in \mathcal{L}(L_2(\mathcal{D}))$ . Thus,

$$\begin{aligned} \|L^{-1/2}(\tilde{L} - L)L^{-1/2}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} &= \|L^{-1/2}M_{\delta_{\kappa^2}}L^{1/2}L^{-1}\|_{\mathcal{L}_2(L_2(\mathcal{D}))} \\ &\geq \|L^{-1/2}M_{\delta_{\kappa^2}^{-1}}L^{1/2}\|_{\mathcal{L}(L_2(\mathcal{D}))}^{-1}\|L^{-1}\|_{\mathcal{L}_2(L_2(\mathcal{D}))}. \end{aligned}$$

The asymptotic behavior (4.4) implies that  $\|L^{-1}\|_{\mathcal{L}_2(L_2(\mathcal{D}))}^2 = \sum_{j \in \mathbb{N}} \lambda_j^{-2} \geq C_{\lambda}^{-2} \sum_{j \in \mathbb{N}} j^{-1} = \infty$  for  $d \geq 4$  and, hence,  $L^{-1/2}\tilde{L}L^{-1/2} - \text{Id}_{L_2(\mathcal{D})} = L^{-1/2}(\tilde{L} - L)L^{-1/2} \notin \mathcal{L}_2(L_2(\mathcal{D}))$ .

**Step 2a:** Suppose now that  $\emptyset \neq \mathcal{D}_0 \in \mathcal{D}$  is an open ball  $\mathcal{D}_0 := B(s_0, r_0)$  with center  $s_0 \in \mathcal{D}$  and radius  $r_0 \in \mathbb{R}_+$  such that  $\delta^+(s) \geq \delta_0 \in \mathbb{R}_+$  for all  $s \in \overline{\mathcal{D}_0}$ . Then, the self-adjoint compact operator  $L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2} \in \mathcal{K}(L_2(\mathcal{D}))$  has infinitely many positive eigenvalues  $\mu_1^+ \geq \mu_2^+ \geq \dots > 0$  that are bounded from below by those of the compact operator  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2} \in \mathcal{K}(L_2(\mathcal{D}_0))$ , where  $L_0: \mathcal{D}(L_0) \subset L_2(\mathcal{D}_0) \rightarrow L_2(\mathcal{D}_0)$  is defined as in (4.2) with respect to the spatial domain  $\mathcal{D}_0 \in \mathcal{D}$  and the coefficients  $\mathbf{a}|_{\overline{\mathcal{D}_0}}$  and  $\kappa|_{\overline{\mathcal{D}_0}}$ . This follows from the min-max theorem, see e.g. [15, Theorem X.4.3], showing that the eigenvalues  $\tilde{\mu}_1^+ \geq \tilde{\mu}_2^+ \geq \dots > 0$  of the positive operator  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$  satisfy

$$\begin{aligned} 0 < \tilde{\mu}_n^+ &= \max_{\substack{U_0 \subset L_2(\mathcal{D}_0), \\ \dim(U_0)=n}} \min_{w_0 \in U_0 \setminus \{0\}} \frac{(L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}w_0, w_0)_{L_2(\mathcal{D}_0)}}{(w_0, w_0)_{L_2(\mathcal{D}_0)}} \\ &= \max_{\substack{V_0 \subset H_0^1(\mathcal{D}_0), \\ \dim(V_0)=n}} \min_{v_0 \in V_0 \setminus \{0\}} \frac{(M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}v_0, v_0)_{L_2(\mathcal{D}_0)}}{\langle L_0v_0, v_0 \rangle}, \end{aligned}$$

where we also used that  $\dot{H}_{L_0}^1 \cong H_0^1(\mathcal{D}_0)$ . If  $\bar{v}_0: \mathcal{D} \rightarrow \mathbb{R}$  denotes the zero extension of  $v_0: \mathcal{D}_0 \rightarrow \mathbb{R}$ , then  $\bar{v}_0 \in H_0^1(\mathcal{D})$  holds if and only if  $v_0 \in H_0^1(\mathcal{D}_0)$ , cf. [1, Theorem 5.29]. Consequently, if we define the closed subspace  $\mathcal{V}_0 := \{v \in H_0^1(\mathcal{D}) \mid \exists v_0 \in H_0^1(\mathcal{D}_0) \text{ such that } v = \bar{v}_0\} \subset H_0^1(\mathcal{D}) \cong \dot{H}_L^1$ , we find

$$\begin{aligned} 0 < \tilde{\mu}_n^+ &= \max_{\substack{V \subset \mathcal{V}_0, \\ \dim(V)=n}} \min_{v \in V \setminus \{0\}} \frac{(M_{\delta_{\kappa^2}}v, v)_{L_2(\mathcal{D})}}{\langle Lv, v \rangle} \leq \max_{\substack{V \subset H_0^1(\mathcal{D}), \\ \dim(V)=n}} \min_{v \in V \setminus \{0\}} \frac{(M_{\delta_{\kappa^2}}v, v)_{L_2(\mathcal{D})}}{(L^{1/2}v, L^{1/2}v)_{L_2(\mathcal{D})}} \\ &= \max_{\substack{U \subset L_2(\mathcal{D}), \\ \dim(U)=n}} \min_{w \in U \setminus \{0\}} \frac{(L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2}w, w)_{L_2(\mathcal{D})}}{(w, w)_{L_2(\mathcal{D})}} = \mu_n^+. \end{aligned}$$

We conclude that, if  $\delta_{\kappa^2}(s) = \delta^+(s) \geq \delta_0 > 0$  for all  $s \in \mathcal{D}_0$ , then  $L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2} \in \mathcal{K}(L_2(\mathcal{D}))$  has infinitely many positive eigenvalues  $\{\mu_n^+\}_{n \in \mathbb{N}}$  satisfying  $\mu_n^+ \geq \tilde{\mu}_n^+$ , where  $\{\tilde{\mu}_n^+\}_{n \in \mathbb{N}}$  are the positive eigenvalues of  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$ .

**Step 2b:** Suppose next that  $\emptyset \neq \mathcal{D}_0 \in \mathcal{D}$  is an open ball  $\mathcal{D}_0 := B(s_0, r_0)$  with center  $s_0 \in \mathcal{D}$  and radius  $r_0 \in \mathbb{R}_+$  such that  $\delta^-(s) \geq \delta_0 \in \mathbb{R}_+$  for all  $s \in \overline{\mathcal{D}_0}$ . Then, as in **Step 2a** we find that the operator  $L^{-1/2}M_{-\delta_{\kappa^2}}L^{-1/2} \in \mathcal{K}(L_2(\mathcal{D}))$  has infinitely many positive eigenvalues  $\{\mu_n^-\}_{n \in \mathbb{N}}$  bounded from below by those of  $L_0^{-1/2}M_{-\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$  denoted by  $\{\tilde{\mu}_n^-\}_{n \in \mathbb{N}}$ .

**Step 3:** Assume that  $\kappa^2 \neq \bar{\kappa}^2$ . Then there exist  $s_0 \in \mathcal{D}$  and  $r_0, \delta_0 \in \mathbb{R}_+$  such that  $B(s_0, r_0) \in \mathcal{D}$  and such that **a)**  $\delta^+(s) \geq \delta_0$  or **b)**  $\delta^-(s) \geq \delta_0$  for all  $s \in \overline{\mathcal{D}_0}$ . By **Step 2** the operator  $L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2}$  has in case **a)** infinitely many positive eigenvalues  $\{\mu_n^+\}_{n \in \mathbb{N}}$  which are bounded from below by  $\{\tilde{\mu}_n^+\}_{n \in \mathbb{N}}$ , i.e., by those of  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$ , and in case **b)** infinitely many negative eigenvalues  $\{-\mu_n^-\}_{n \in \mathbb{N}}$  which are bounded from above by  $\{-\tilde{\mu}_n^-\}_{n \in \mathbb{N}}$ , i.e., by those of  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$ . By **Step 1** the eigenvalues of  $L_0^{-1/2}M_{\delta_{\kappa^2}|_{\mathcal{D}_0}}L_0^{-1/2}$  are not square-summable and by **Step 2** neither those of  $L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2}$  can be, i.e.,  $L^{-1/2}M_{\delta_{\kappa^2}}L^{-1/2} \notin \mathcal{L}_2(L_2(\mathcal{D}))$ . □

We now can combine the foregoing Lemmas 4.8, 4.9 and 4.10 with the general results on Gaussian measures with fractional-order covariance operators of Section 2 to deduce the following result on equivalence of Gaussian measures of generalized Whittle–Matérn type.

**Theorem 4.11.** *Let  $d \in \mathbb{N}$ ,  $\beta, \tilde{\beta} \in (d/4, \infty)$  be such that  $2\beta \notin \mathfrak{E}$ , with  $\mathfrak{E}$  as in (4.6), and suppose Assumption 4.1.III. Let  $L$  and  $\tilde{L}$  be defined as in (4.2), with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively, where each of the tuples  $(\mathbf{a}, \kappa)$  and  $(\tilde{\mathbf{a}}, \tilde{\kappa})$  fulfills Assumptions 4.1.I–II. Assume that  $m, \tilde{m} \in L_2(\mathcal{D})$  and let the Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  be defined according to (4.5).*

- I. *In dimension  $d \leq 3$ , the Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  are equivalent if and only if  $\beta = \tilde{\beta}$ ,  $m - \tilde{m} \in \dot{H}_L^{2\beta}$ ,  $\mathbf{a} = \tilde{\mathbf{a}}$ , and the boundary conditions (4.16) hold for every  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ .*
- II. *In dimension  $d \geq 4$ , the Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  are equivalent if and only if  $\beta = \tilde{\beta}$ ,  $m - \tilde{m} \in \dot{H}_L^{2\beta}$ ,  $\mathbf{a} = \tilde{\mathbf{a}}$ , and  $\kappa^2 = \tilde{\kappa}^2$ .*

**Proof.** For the derivation we apply the Feldman–Hájek theorem, see Theorem B.1 in the Supplementary Material [6]. To this end, we let  $C = L^{-2\beta}$  and  $\tilde{C} = \tilde{L}^{-2\tilde{\beta}}$  denote the covariance operators corresponding to  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , respectively. By Theorem 4.7 the Cameron–Martin spaces  $C(L_2(\mathcal{D})) = \dot{H}_L^{2\beta}$  and  $\tilde{C}(L_2(\mathcal{D})) = \dot{H}_{\tilde{L}}^{2\tilde{\beta}}$  are norm equivalent spaces (and thus condition (i) of Theorem B.1 is fulfilled) if and only if  $\beta = \tilde{\beta}$  and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ . Next we note that condition (ii) of Theorem B.1 is equivalent to requiring that  $m - \tilde{m} \in \dot{H}_L^{2\beta}$ .

Assuming that  $\beta = \tilde{\beta}$  with  $2\beta \notin \mathfrak{E}$ , we complete the proof by showing that conditions (i) and (iii) of Theorem B.1 hold simultaneously, i.e.,  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and the operator  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$  is Hilbert–Schmidt on  $L_2(\mathcal{D})$  I. in dimension  $d \leq 3$  if and only if  $\mathbf{a} = \tilde{\mathbf{a}}$  and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ ; and II. for  $d \geq 4$  if and only if  $\mathbf{a} = \tilde{\mathbf{a}}$  and  $\kappa^2 = \tilde{\kappa}^2$ .

I. If  $d \leq 3$ ,  $\mathbf{a} = \tilde{\mathbf{a}}$ , and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ , then  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$  is Hilbert–Schmidt on  $L_2(\mathcal{D})$  by Lemma 4.8. Conversely, if  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})} \in \mathcal{L}_2(L_2(\mathcal{D}))$ , then by Lemma 2.1(i) for every  $\gamma \in [-\beta, \beta]$  also the operator  $\tilde{L}^\gamma L^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\gamma} \tilde{L}^{2\gamma} L^{-\gamma} - \text{Id}_{L_2(\mathcal{D})}$  is a Hilbert–Schmidt operator on  $L_2(\mathcal{D})$ . Since  $2\beta \notin \mathfrak{E}$  is assumed, by Theorem 4.7 the conditions (4.16) have to be satisfied for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ . Furthermore, the choice  $\gamma = 1/4$  shows that  $L^{-1/4} \tilde{L}^{1/2} L^{-1/4} - \text{Id}_{L_2(\mathcal{D})}$  is Hilbert–Schmidt and, thus, compact on  $L_2(\mathcal{D})$ . Lemma 4.9 (with  $c = 1$ ) therefore implies then that  $\mathbf{a} = \tilde{\mathbf{a}}$  has to hold.

II. If  $d \geq 4$ ,  $\mathbf{a} = \tilde{\mathbf{a}}$  and  $\kappa^2 = \tilde{\kappa}^2$ , then  $L = \tilde{L}$  so that the isomorphism property of  $\tilde{L}^\beta L^{-\beta}$  and the Hilbert–Schmidt property of  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})}$  are trivial. Conversely, if  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - \text{Id}_{L_2(\mathcal{D})} \in \mathcal{L}_2(L_2(\mathcal{D}))$  in dimension  $d \geq 4$ , then  $\beta > d/4 \geq 1$  and by Lemma 2.1(i) also the operators  $L^{-1/4} \tilde{L}^{1/2} L^{-1/4} - \text{Id}_{L_2(\mathcal{D})}$  as well as  $L^{-1/2} \tilde{L} L^{-1/2} - \text{Id}_{L_2(\mathcal{D})}$  are Hilbert–Schmidt (and, thus, compact) on  $L_2(\mathcal{D})$ . By Lemma 4.9  $\mathbf{a} = \tilde{\mathbf{a}}$  follows and, subsequently, Lemma 4.10 shows that  $\kappa^2 = \tilde{\kappa}^2$ . □

#### 4.4. Uniformly asymptotically optimal linear prediction

In contrast to equivalence of the Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , the necessary and sufficient conditions for uniformly asymptotically optimal linear prediction (2.10), (2.11) when misspecifying  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  by  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  derived in this subsection will not depend on the dimension  $d$  of the spatial domain  $\mathcal{D} \subset \mathbb{R}^d$ . The key to prove this result is the next lemma.

**Lemma 4.12.** *Let  $d \in \mathbb{N}$ ,  $c \in \mathbb{R}_+$ , and let  $\beta \in (d/4, \infty)$  be such that  $2\beta \notin \mathfrak{E}$ , where  $\mathfrak{E}$  is as in (4.6). In addition, suppose Assumption 4.1.III and let the operators  $L, \tilde{L}$  be defined as in (4.2) with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively, where  $\mathbf{a}$  fulfills Assumption 4.1.I,  $c\mathbf{a} = \tilde{\mathbf{a}}$ , and  $\kappa, \tilde{\kappa}$  are such that Assumption 4.1.II is satisfied and (4.16) holds for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ . Then,  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism on  $L_2(\mathcal{D})$  and  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - c^{2\beta} \text{Id}_{L_2(\mathcal{D})} \in \mathcal{K}(L_2(\mathcal{D}))$ .*

**Proof.** By Theorem 4.7  $\tilde{L}^\gamma L^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  for all  $\gamma \in [-\beta, \beta]$ . To prove compactness of  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - c^{2\beta} \text{Id}_{L_2(\mathcal{D})}$ , similarly as in the proof of Lemma 4.8, we distinguish two cases, namely **Case I:**  $d \in \{1, 2, 3\}$ ,  $\beta \in (d/4, 1)$  and **Case II:**  $\beta \in [1, \infty)$ .

**Case I:** If  $d \in \{1, 2, 3\}$  and  $\beta \in (d/4, 1)$ , then we use the identity

$$\begin{aligned} L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - c^{2\beta} \text{Id}_{L_2(\mathcal{D})} &= \frac{1}{2} L^{-\beta} (\tilde{L}^\beta + c^\beta L^\beta) (\tilde{L}^\beta - c^\beta L^\beta) L^{-\beta} \\ &\quad + \frac{1}{2} [L^{-\beta} (\tilde{L}^\beta + c^\beta L^\beta) (\tilde{L}^\beta - c^\beta L^\beta) L^{-\beta}]^*. \end{aligned} \tag{4.21}$$

Clearly,  $L^{-\beta} \tilde{L}^\beta \in \mathcal{L}(L_2(\mathcal{D}))$  is bounded, since  $\tilde{L}^\beta L^{-\beta}$  is an isomorphism. Furthermore, since  $(\tilde{L} - cL)\psi = \delta_{c, \kappa^2} \psi$ , where  $\delta_{c, \kappa^2} := \tilde{\kappa}^2 - c\kappa^2 \in C^\infty(\overline{\mathcal{D}})$ , we find that  $\tilde{L} - cL \in \mathcal{L}(L_2(\mathcal{D}))$ . Thus, by Lemma C.1 and Remark C.2 in Appendix C also  $\tilde{L}^\beta - c^\beta L^\beta \in \mathcal{L}(L_2(\mathcal{D}))$  holds. Combining these observations with (4.21) and  $L^{-\beta} \in \mathcal{K}(L_2(\mathcal{D}))$  shows that  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - c^{2\beta} \text{Id}_{L_2(\mathcal{D})} \in \mathcal{K}(L_2(\mathcal{D}))$ .

**Case II:** Define the operator  $L_c := cL$ . Then, also  $\tilde{L}^\gamma L_c^{-\gamma}$  is an isomorphism on  $L_2(\mathcal{D})$  for every  $\gamma \in [-\beta, \beta]$ . By Theorem 4.7, for all  $\eta \in \mathfrak{N}_\beta$ , where  $\mathfrak{N}_\beta$  is as in (2.5), and all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ ,

$$\forall v \in \dot{H}_{L_c}^{2\eta} = \dot{H}_L^{2\eta} : (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{c, \kappa^2} v) = 0 \text{ in } L_2(\partial\mathcal{D}).$$

We pick  $\varepsilon_0 \in (0, 2)$  such that  $2\eta - \varepsilon_0 \notin \mathfrak{E}$  for all  $\eta \in \mathfrak{N}_\beta$ , and we fix  $\eta \in \mathfrak{N}_\beta$ ,  $\psi \in \dot{H}_L^{2\eta - \varepsilon_0}$ , and  $\delta \in \mathbb{R}_+$ . By density of  $\dot{H}_L^{2\eta}$  in  $\dot{H}_L^{2\eta - \varepsilon_0}$ , there exists  $v_\delta \in \dot{H}_L^{2\eta}$  such that  $\|\psi - v_\delta\|_{2\eta - \varepsilon_0, L} < \delta$ . Furthermore, by Lemma 4.3 on  $\dot{H}_L^{2\eta - \varepsilon_0}$  the norm  $\|\cdot\|_{2\eta - \varepsilon_0, L}$  is equivalent to the Sobolev norm  $\|\cdot\|_{H^{2\eta - \varepsilon_0}(\mathcal{D})}$ .

Thus, by the trace theorem, Theorem A.3 in Appendix A, and by noting that  $5/2 - \varepsilon_0 \in (1/2, 5/2)$ , for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ , we find that

$$\begin{aligned} \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{c, \kappa^2} \psi)\|_{L_2(\partial\mathcal{D})} &= \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{c, \kappa^2} (\psi - v_\delta))\|_{L_2(\partial\mathcal{D})} \\ &\leq C \|(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{c, \kappa^2} (\psi - v_\delta))\|_{H^{5/2 - \varepsilon_0}(\mathcal{D})} \leq \widehat{C} \|\psi - v_\delta\|_{H^{2\eta - \varepsilon_0}(\mathcal{D})} < C' \delta, \end{aligned}$$

where the constants  $C, \widehat{C}, C' \in \mathbb{R}_+$  are independent of  $\delta, v_\delta$  and  $\psi$ . Since  $\psi \in \dot{H}_L^{2\eta - \varepsilon_0}$  and  $\delta \in \mathbb{R}_+$  were arbitrary, we thus find that, for every  $\eta \in \mathfrak{N}_\beta$  and all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \eta - 5/4 \rfloor$ ,

$$\forall \psi \in \dot{H}_{L_c}^{2\eta - \varepsilon_0} = \dot{H}_L^{2\eta - \varepsilon_0} : (\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))^j (\delta_{c, \kappa^2} \psi) = 0 \text{ in } L_2(\partial\mathcal{D}). \tag{4.22}$$

Since  $\varepsilon_0 \in (0, 2)$ , the identity (4.22) and the regularity of  $\delta_{c, \kappa^2} \in C^\infty(\overline{\mathcal{D}})$  imply by identifying  $\dot{H}_{L_c}^{2(\eta-1)}$  as in (4.7) that  $B_c := \tilde{L} - cL \in \mathcal{L}(\dot{H}_{L_c}^{2\eta - \varepsilon_0}, \dot{H}_{L_c}^{2(\eta-1)})$  and  $L_c^{\eta-1} B_c L_c^{-\eta + \varepsilon_0/2} \in \mathcal{L}(L_2(\mathcal{D}))$ . Then, we find that  $K_\eta := L_c^{\eta-1} \tilde{L} L_c^{-\eta} - \text{Id}_{L_2(\mathcal{D})} = L_c^{\eta-1} (\tilde{L} - L_c) L_c^{-\eta} = (L_c^{\eta-1} B_c L_c^{-\eta + \varepsilon_0/2}) L_c^{-\varepsilon_0/2} \in \mathcal{K}(L_2(\mathcal{D}))$  for every  $\eta \in \mathfrak{N}_\beta$ , because  $L_c^{-\varepsilon_0/2} = c^{-\varepsilon_0/2} L^{-\varepsilon_0/2}$  is compact on  $L_2(\mathcal{D})$ . Applying Lemma 2.2(ii) (for  $\tilde{A} := \tilde{L}$  and  $A := L_c$ , using  $W_\eta := \text{Id}_{L_2(\mathcal{D})}$  for every  $\eta \in \mathfrak{N}_\beta$ ) finally yields compactness of the operator  $L^{-\gamma} \tilde{L}^{2\gamma} L^{-\gamma} - c^{2\gamma} \text{Id}_{L_2(\mathcal{D})} = c^{2\gamma} (L_c^{-\gamma} \tilde{L}^{2\gamma} L_c^{-\gamma} - \text{Id}_{L_2(\mathcal{D})})$  on  $L_2(\mathcal{D})$  for all  $\gamma \in [-\beta, \beta]$ .  $\square$

**Theorem 4.13.** *Let  $d \in \mathbb{N}$ ,  $\beta, \tilde{\beta} \in (d/4, \infty)$  be such that  $2\beta \notin \mathfrak{E}$ , with  $\mathfrak{E}$  as in (4.6), and let Assumption 4.1.III be satisfied. Suppose that  $L, \tilde{L}$  are defined as in (4.2), with coefficients  $\mathbf{a}, \kappa$  and  $\tilde{\mathbf{a}}, \tilde{\kappa}$ , respectively, where each of the tuples  $(\mathbf{a}, \kappa)$  and  $(\tilde{\mathbf{a}}, \tilde{\kappa})$  fulfills Assumptions 4.1.I–II. Let  $m, \tilde{m} \in L_2(\mathcal{D})$  and the Gaussian measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  and  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$  be defined according to (4.5). In addition, let  $h_n, \tilde{h}_n$  denote the best linear predictors of  $h \in \mathcal{H}$  based on  $\mathcal{H}_n$  and the measures  $\mu_d(m; \beta, \mathbf{a}, \kappa)$  resp.  $\mu_d(\tilde{m}; \tilde{\beta}, \tilde{\mathbf{a}}, \tilde{\kappa})$ , see (2.6)–(2.9). Then, any of the four assertions in (2.10), (2.11) holds for some  $c \in \mathbb{R}_+$  and all  $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^\mu$  if and only if  $\beta = \tilde{\beta}$ ,  $m - \tilde{m} \in \dot{H}_L^{2\beta}$ , the boundary conditions (4.16) hold for every  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ , and there exists a constant  $\hat{c} \in \mathbb{R}_+$  such that  $\hat{c}\mathbf{a} = \tilde{\mathbf{a}}$ .*

**Proof.** By [22, Theorem 3.8 and Lemma B.1] any of the assertions in (2.10), (2.11) holds for some constant  $c \in \mathbb{R}_+$  and all  $\{\mathcal{H}_n\}_{n \in \mathbb{N}} \in \mathcal{S}_{\text{adm}}^\mu$  if and only if (i)  $\dot{H}_L^{2\beta}$  and  $\dot{H}_{\tilde{L}}^{2\tilde{\beta}}$  are norm equivalent Hilbert spaces; (ii)  $m - \tilde{m} \in \dot{H}_L^{2\beta}$ ; and (iii)  $L^{-\beta} \tilde{L}^{2\beta} L^{-\beta} - c^{-1} \text{Id}_{L_2(\mathcal{D})}$  is compact on  $E$ .

By Theorem 4.7  $\dot{H}_L^{2\beta}$  and  $\dot{H}_{\tilde{L}}^{2\tilde{\beta}}$  are norm equivalent if and only if  $\beta = \tilde{\beta}$  and (4.16) holds for every  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ . Assuming that  $\beta = \tilde{\beta}$  with  $2\beta \notin \mathfrak{E}$ , sufficiency of (a) the boundary conditions (4.16) holding for all  $j \in \mathbb{N}_0$  with  $j \leq \lfloor \beta - 5/4 \rfloor$ , combined with (b) the existence of  $\hat{c} \in \mathbb{R}_+$  such that  $\hat{c}\mathbf{a} = \tilde{\mathbf{a}}$ , for conditions (i) and (iii) is proven in Lemma 4.12 (showing in particular that  $c^{-1} = \hat{c}^{2\beta}$ ). Necessity of (a) and (b) follows from Theorem 4.7 and Lemma 4.9. □

### 5. Illustration by simulations

In this section we illustrate the theoretical findings of the previous sections by two different examples of kriging prediction based on misspecified generalized Whittle–Matérn models (1.4), see also (4.1) and (4.2), on  $\mathcal{D} := (0, 1)$ . We first consider a non-fractional model with  $\beta = 1$  and discuss the difference between a misspecification of  $\kappa^2$  and of  $\mathbf{a}$ . We then consider the role of  $\beta$  when misspecifying  $\kappa^2$ . These examples verify, in particular, that one obtains asymptotic optimality even if  $\kappa^2$  is misspecified for  $\beta < 9/4$ . In contrast, when  $\beta > 9/4$ , it is the behavior of  $\kappa^2$  at the boundary  $\partial\mathcal{D} = \{0, 1\}$  of the domain  $\mathcal{D} = (0, 1)$  that determines whether asymptotic optimality is achieved or not, see Table 1. The results are implemented in MATLAB using the `ppfem` package [3] for discretizing the models.

To facilitate interpreting the parameters, we make a small adjustment to the Whittle–Matérn model (1.4) by including a constant  $\tau \in \mathbb{R}_+$  which scales the variance of the solution:

$$(-\nabla \cdot (\mathbf{a}\nabla) + \kappa^2)^\beta (\tau Z) = \mathcal{W} \quad \text{in } \mathcal{D} = (0, 1). \tag{5.1}$$

Note that this constant has no effect on the kriging prediction.

#### 5.1. The difference between $\kappa^2$ and $\mathbf{a}$

Consider (5.1) with  $\beta = 1$ ,  $\mathbf{a} \equiv 1$ ,  $\kappa^2 \equiv 1200$ , and  $\tau = \frac{1}{2}\kappa^{-3/2}$ . These choices result in a process  $Z$  with practical correlation range 0.1 and a variance of approximately 1 at the center of the domain, see (1.3).

We approximate the solution  $Z: [0, 1] \times \Omega \rightarrow \mathbb{R}$  of (5.1) using a finite element method (FEM) with  $N = 1000$  equally spaced continuous, piecewise linear basis functions  $\{\varphi_k\}_{k=1}^N$ , aka. “hat functions”. The resulting approximation can be written as  $Z(s) \approx \sum_{k=1}^N z_k \varphi_k(s)$ , where the distribution of the weights  $\{z_k\}_{k=1}^N$  is zero-mean multivariate Gaussian with covariance matrix  $\mathbf{C} = \mathbf{L}^{-1}\mathbf{M}\mathbf{L}^{-1}$ . The matrix  $\mathbf{L}$  has elements  $L_{jk} = a_L(\varphi_j, \varphi_k)$ , where  $a_L(\cdot, \cdot)$  denotes the bilinear form induced by  $L$ , see

(4.3) in Subsection 4.1, and  $\mathbf{M}$  is the mass matrix (aka. Gramian) with elements  $M_{jk} = (\varphi_j, \varphi_k)_{L_2(\mathcal{D})}$ . For details on the implementation, such as the assembling of the matrices, see [23] or [7].

To evaluate the effect of misspecifying the covariance function, the predictive performance of the correct model is compared with two misspecified models. For both misspecified models, we use the correct values of  $\beta, \tau$ , and we set

$$(\kappa^2(s), \mathbf{a}(s)) = \begin{cases} (1200f(s)^{-1}, 1) & \text{for model 1,} \\ (1200, f(s)) & \text{for model 2,} \end{cases} \quad s \in \overline{\mathcal{D}} = [0, 1]. \tag{5.2}$$

Here,  $f(s) = 1 + \frac{1}{2} \operatorname{erf}\left(\frac{\delta(s-0.5)}{\sqrt{2}}\right)$  is a sigmoid function defined through the error function, and  $\delta \in \mathbb{R}_+$  is a parameter that determines the rate of change of  $f(s)$  at  $s = 0.5$ . Thus, for the first model the coefficient  $\kappa^2$ , which is constant in the true model, is misspecified by a function, whereas in the second model this scenario applies to the coefficient  $\mathbf{a}$ . Note that, for both models,  $\kappa^2(s)$  and  $\mathbf{a}(s)$  attain the correct values at  $s = 0.5$ . The two misspecified models are approximated by means of a FEM approximation with the same basis functions as used for the true model.

We consider kriging prediction in two different scenarios. In both scenarios, we use

$$\mathcal{E}_n(h) := \frac{\mathbb{E}[(\tilde{h}_n - h)^2]}{\mathbb{E}[(h_n - h)^2]} - 1,$$

as a measure of efficiency of the best linear predictor obtained by a misspecified model. The quantity  $\mathcal{E}_n(h)$  is always nonnegative and should converge to zero if the misspecified model provides asymptotically optimal linear prediction, see Proposition 2.6 and Theorem 4.13.

In the first scenario, we predict integral values of  $Z$ . Specifically, for  $\ell \in \mathbb{N}$ , let  $I_\ell := (Z, e_\ell)_{L_2(\mathcal{D})}$  be the integral over the product of the process with  $e_\ell(s) := \sqrt{2} \sin(\ell\pi s)$ , which is the  $\ell$ -th eigenfunction of the (negative) Dirichlet Laplacian  $-\Delta$  on  $\mathcal{D} = (0, 1)$ . In order to evaluate  $I_\ell$ , we use the FEM approximation  $I_\ell \approx \sum_{k=1}^N z_k (e_\ell, \varphi_k)_{L_2(\mathcal{D})}$  and evaluate the integral  $\Phi_{\ell k} = (e_\ell, \varphi_k)_{L_2(\mathcal{D})}$  by means of Gauss–Legendre quadrature. Collecting these elements in a matrix  $\Phi$  we find that the joint distribution of  $(I_1, \dots, I_N)$  is multivariate Gaussian with mean zero and covariance matrix  $\Sigma = \Phi \mathbf{C} \Phi^\top$ . Given  $I_1, \dots, I_n$ , we then predict  $h = I_\ell$  for all  $\ell \in \{n+1, \dots, N\}$ . The variance of the error of this predictor can be obtained as  $\mathbb{E}[(h_n - h)^2] = \Sigma_{\ell, \ell} - \Sigma_{\ell, 1:n} \Sigma_{1:n, 1:n}^{-1} \Sigma_{\ell, 1:n}^\top$ . Here  $\Sigma_{\ell, 1:n}$  denotes the first  $n$  elements of the  $\ell$ -th row of  $\Sigma$  and  $\Sigma_{1:n, 1:n}$  is the  $n \times n$  sub-matrix corresponding to the  $n$  observations. If we let  $\tilde{\mathbf{C}}$  denote the covariance matrix for the weights of a model with misspecified parameters and set  $\tilde{\Sigma} = \Phi \tilde{\mathbf{C}} \Phi^\top$ , we similarly obtain that

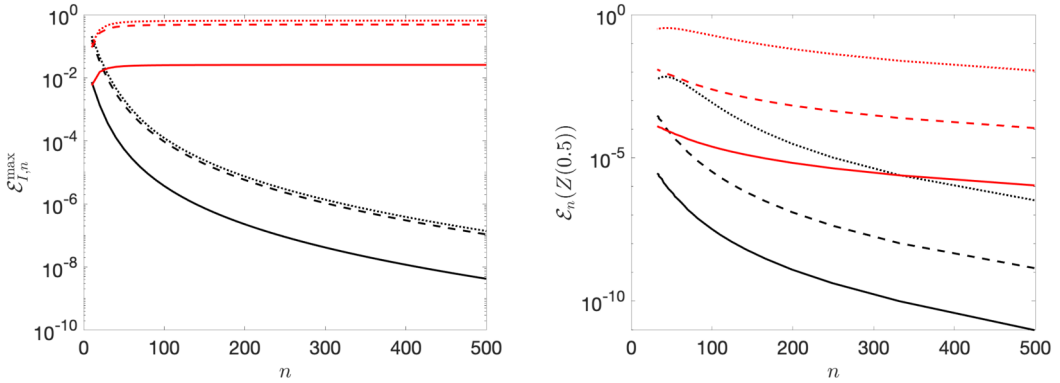
$$\mathbb{E}[(\tilde{h}_n - h)^2] = \Sigma_{\ell, \ell} + \tilde{\Sigma}_{\ell, 1:n} \tilde{\Sigma}_{1:n, 1:n}^{-1} \Sigma_{1:n, 1:n} \tilde{\Sigma}_{1:n, 1:n}^{-1} \tilde{\Sigma}_{\ell, 1:n}^\top - 2 \Sigma_{\ell, 1:n} \tilde{\Sigma}_{1:n, 1:n}^{-1} \tilde{\Sigma}_{\ell, 1:n}^\top.$$

The left panel of Figure 1 shows

$$\mathcal{E}_{I, n}^{\max} := \max\{\mathcal{E}_{I, n}^\ell : n+1 \leq \ell \leq N\}, \quad \mathcal{E}_{I, n}^\ell := \mathcal{E}_n(I_\ell), \quad \ell \in \{n+1, \dots, N\}, \tag{5.3}$$

as a function of  $n$  for both misspecified models, where we consider values for  $n$  up to 500, so that the maximum in (5.3) is taken over at least 500 elements for each  $n$ . This error is computed for three different values of  $\delta$ , namely  $\delta \in \{1, 10, 100\}$ , where a larger value of  $\delta$  intuitively should cause a bigger error for the misspecified model. We can clearly see that model 2 does not provide asymptotically optimal linear prediction in this scenario, but model 1 does. This holds for each of the three different values of  $\delta$ , and is in line with our theoretical findings: Theorem 4.13 (see also Table 1) shows that only the model with misspecified  $\kappa^2$  should provide asymptotically optimal linear prediction.





**Figure 1.** The results for model 1 (black) and model 2 (red) for the first example (5.2) with integral observations (left) and point observations (right). Solid lines correspond to  $\delta = 1$ , dashed to  $\delta = 10$ , and dotted to  $\delta = 100$ .

As a second scenario, we let  $h = Z(s_0)$  with  $s_0 = 0.5$  and compute predictions of  $h$  based on observations of  $Z(s)$  at  $n$  locations  $s_1, s_2, \dots$  in  $\mathcal{D} = (0, 1)$  chosen as  $s_{2j} = s_0 + j\delta_o$  and  $s_{2j-1} = s_0 - j\delta_o$  for  $j \in \mathbb{N}$ . Here  $\delta_o \in (0, 1/2)$  is a constant that determines the distance between the observations. The only difference in the calculations in this case is that the matrix  $\Phi$  now contains the elements  $\Phi_{\ell k} = \varphi_k(s_{\ell-1})$ . We again compute predictions based on both misspecified models and use  $\mathcal{E}_n(Z(s_0))$  to measure the accuracy. The right panel of Figure 1 shows the results as functions of  $n$  for the two different models and the three different values of  $\delta$ . We can now see that model 2 has a larger error compared to model 1. However, also the error of model 2 seem to converge to zero in this case, although at a worse rate compared to model 1.

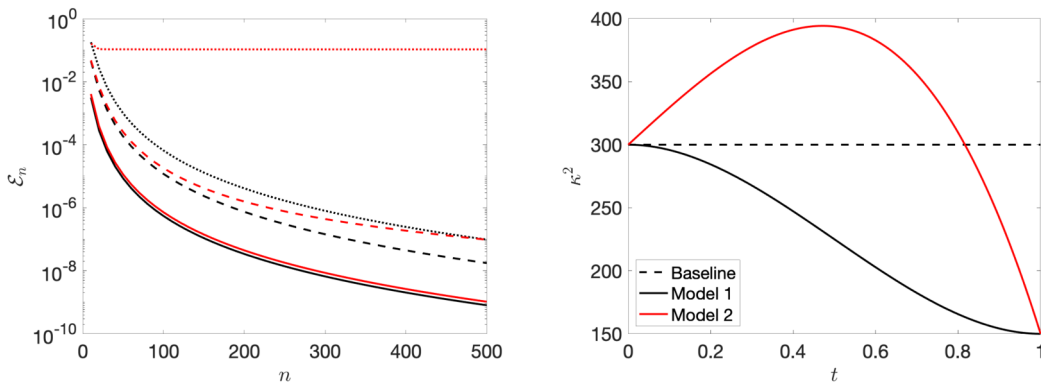
We recall that Theorem 4.13 in Subsection 4.4 specifies necessary and sufficient conditions for *uniform* asymptotic optimality of linear prediction based on misspecified Whittle–Matérn models. Here, uniformity means that the supremum of  $\mathcal{E}_n(h)$  taken over all  $h \in \mathcal{H}_n = \{h \in \mathcal{H} : \mathbb{E}[(h_n - h)^2] > 0\}$  should converge to zero as  $n \rightarrow \infty$ , see (2.10). In particular, the outcomes of the second example, where one specific  $h \in \mathcal{H}$  is fixed, do not contradict the results of Subsection 4.4. Interestingly, they suggest, however, that the conditions of Theorem 4.13 and of [22, Assumption 3.3] are *not necessary* for asymptotically optimal linear prediction when predicting the random field at a single location.

### 5.2. The effect of the smoothness parameter

We again consider the Whittle–Matérn model (5.1) on  $\mathcal{D} = (0, 1)$ , this time for  $\mathbf{a} \equiv 1$  and  $\beta \in \{1, 2, 3\}$ . For the approximation of the solution  $Z$ , we use a finite element discretization with  $N = 2000$  equally spaced hat functions as basis functions. For  $\beta = 2$  and  $\beta = 3$  we follow the iterative approach of [23] and [7]. That is, we replace the matrix  $\mathbf{L}$  (corresponding to the operator  $L$  for  $\beta = 1$ ) by  $\mathbf{L}\mathbf{M}^{-1}\mathbf{L}$  when  $\beta = 2$  and by  $\mathbf{L}\mathbf{M}^{-1}\mathbf{L}\mathbf{M}^{-1}\mathbf{L}$  when  $\beta = 3$  (corresponding to the operators  $L^2$  and  $L^3$ , respectively).

As a baseline model, we consider (5.1) with  $\mathbf{a} \equiv 1$ ,  $\tau = (4\pi)^{-1/4} \kappa^{1/2-2\beta} (\Gamma(2\beta - 1/2)/\Gamma(2\beta))^{1/2}$ , and  $\kappa^2 \equiv 100(4\beta - 1)$ , so that the model has practical correlation range 0.2 and variance close to 1 at the center of the domain, cf. (1.3). For  $\beta \in \{1, 2, 3\}$ , we consider two different models of the form (5.1), where we keep  $\mathbf{a} \equiv 1$  and the constant  $\tau$  fixed to their correct values but misspecify  $\kappa^2$  by

$$\kappa^2(s) = 100(4\beta - 1) \cdot \begin{cases} 1 - 1.5s^2 + s^3 & \text{for model 1,} \\ 1 + s - 1.5s^3 & \text{for model 2,} \end{cases} \quad s \in \overline{\mathcal{D}} = [0, 1], \quad (5.4)$$



**Figure 2.** Left: the results for model 1 (black) and model 2 (red) in the second example (5.4), with  $\beta = 1$  (solid),  $\beta = 2$  (dashed), and  $\beta = 3$  (dotted). Right:  $\kappa^2$  for the two models in (5.4) when  $\beta = 1$ .

see the right panel of Figure 2. In both cases,  $\kappa^2(s)$  takes the correct value at  $s = 0$  and half of the correct value at  $s = 1$ . The main difference between the two models is that the derivative of  $\kappa^2$  vanishes on the boundary for model 1, but not for model 2. Because of this, model 1 induces the same boundary conditions as the baseline model, whereas model 2 changes the boundary condition when  $\beta = 3$ , cf. (4.7) and Theorem 4.7. From the results of Subsections 4.1 and 4.4 we know that the behavior of  $\kappa^2$  for the two alternative models implies that model 1 will provide uniformly asymptotically optimal linear prediction for all values of  $\beta \in \{1, 2, 3\}$  whereas model 2 only will do so for  $\beta = 1$  and  $\beta = 2$  (see Table 1, where  $c = 1$  and  $\delta_{c, \kappa^2}$  has a derivative that does not vanish at the boundary  $s \in \{0, 1\}$ ).

To investigate this, we again consider predicting the integral values  $I_\ell = (Z, e_\ell)_{L_2(\mathcal{D})}$ . Given observations of  $I_1, \dots, I_n$  we predict  $h = I_\ell$  for  $\ell \in \{n + 1, \dots, N\}$  and compute  $\mathcal{E}_{I,n}^{\max}$  as the largest error among these predictions, see (5.3). Figure 2 shows  $\mathcal{E}_{I,n}^{\max}$  as a function of  $n$  for both misspecified models in the three cases  $\beta \in \{1, 2, 3\}$ . The figure verifies that both misspecified models provide asymptotically optimal predictions when  $\beta \in \{1, 2\}$  but, for  $\beta = 3$ , only the predictions based on model 1 behave asymptotically optimal.

## 6. Discussion

In the general setting of Gaussian measures with fractional-order covariance operators on separable Hilbert spaces, we have derived necessary and sufficient conditions for I. equivalence of Gaussian measures in Proposition 2.3, and II. uniform asymptotic optimality of linear (kriging) prediction based on misspecified Gaussian measures in Proposition 2.6. These conditions are formulated in terms of the non-fractional base operators, and are therefore in many situations simpler to verify than those for I. as given by the Feldman–Hájek theorem and those for II. as stated in [22, Assumption 3.3]. As a first explicit example, we have applied these results to classical Whittle–Matérn fields, see Corollary 3.3.

In the second part of the manuscript, we adopted the general results to derive necessary and sufficient conditions for I. and II. in terms of the (possibly function-valued) parameters of generalized Whittle–Matérn fields on bounded Euclidean domains, see (4.1), (4.2) and (4.5). The outcomes of Theorems 4.7, 4.11 and 4.13 cover the whole range of admissible fractional orders  $\beta \in (d/4, \infty)$  except for the cases  $2\beta \in \mathfrak{E}$ , i.e.,  $\beta \in \{k + 1/4 : k \in \mathbb{N}\}$ , see also Table 1. For ease of presentation, we refrained from detailing the results for  $2\beta \in \mathfrak{E}$  and we will now briefly comment on this situation. In the case that  $r \in \mathfrak{E}$  belongs to the discrete exception set (4.6), on  $\dot{H}_L^r$  the Sobolev norm  $\|\cdot\|_{H^r(\mathcal{D})}$  will not be

equivalent to the norm  $\|\cdot\|_{r,L} = \|L^{r/2} \cdot\|_{L_2(\mathcal{D})}$  defined through the fractional power operator  $L^{r/2}$ , as the topology on  $\dot{H}_L^r$  is strictly finer than that on  $H^r(\mathcal{D})$ . It is well-known (see e.g. [24, Theorem 11.7 in Chapter 1]) that, for instance, for  $r = 1/2$  the norm  $\|\cdot\|_{1/2,L}$  is equivalent to the norm

$$\|v\|_{H_0^{1/2}(\mathcal{D})} := (\|v\|_{H^{1/2}(\mathcal{D})}^2 + \|\rho^{-1/2}v\|_{L_2(\mathcal{D})}^2)^{1/2},$$

where  $\rho \in C^\infty(\overline{\mathcal{D}})$  is a function which is positive in the interior  $\mathcal{D}$  and for which the limit  $\lim_{s \rightarrow s_0} \frac{\rho(s)}{\text{dist}(s, \partial\mathcal{D})}$  exists and is not zero for all  $s_0 \in \partial\mathcal{D}$ , where  $\text{dist}(s, \partial\mathcal{D})$  denotes the distance of  $s$  to the boundary  $\partial\mathcal{D}$ . For example, in the case that  $\beta = 5/4$  and  $2\beta = 5/2 \in \mathfrak{C}$ , we therefore expect the Cameron–Martin spaces of the Gaussian Whittle–Matérn measures  $\mu(0; \beta, \mathbf{a}, \kappa)$  and  $\mu(0; \beta, \mathbf{a}, \bar{\kappa})$ , see (4.5), to be isomorphic with equivalent norms for any choice of the coefficients  $\kappa, \bar{\kappa} \in C^\infty(\overline{\mathcal{D}})$  since  $\delta_{\kappa^2} = \bar{\kappa}^2 - \kappa^2 \in C^\infty(\overline{\mathcal{D}})$  and  $\rho^{-1/2}\delta_{\kappa^2}v \in L_2(\mathcal{D})$  for all  $v \in \dot{H}_L^{5/2} \cup \dot{H}_L^{3/2} \subset H_0^{1/2}(\mathcal{D})$ . For  $\beta = 9/4$ , we expect this to hold if and only if

$$(\kappa^2 - \nabla \cdot (\mathbf{a}\nabla))(\delta_{\kappa^2}v) \in H_0^{1/2}(\mathcal{D}) \quad \text{and} \quad (\bar{\kappa}^2 - \nabla \cdot (\mathbf{a}\nabla))(\delta_{\kappa^2}\tilde{v}) \in H_0^{1/2}(\mathcal{D}),$$

for every  $v \in \dot{H}_L^{9/2}$  and all  $\tilde{v} \in \dot{H}_L^{9/2}$ . Similarly, as in (4.17) and (4.18) this results in the condition  $\rho^{-1/2}(\mathbf{a}\nabla\delta_{\kappa^2}) \cdot \nabla v \in L_2(\mathcal{D})$  for all  $v \in \dot{H}_L^{9/2} \cup \dot{H}_L^{7/2}$ . This means that  $\mathbf{a}\nabla\delta_{\kappa^2}$  has to satisfy a certain decay behavior towards to the boundary  $\partial\mathcal{D}$ . Analogous conditions can also be derived for  $\beta \in \{13/4, 17/4, \dots\}$  and for the case that  $\mathbf{a} \neq \bar{\mathbf{a}}$ . Furthermore, although we have addressed only Gaussian measures in this work, the results for II. extend to non-Gaussian processes, since the kriging predictor solely depends on the first two moments of the process.

As a natural extension of the results of this work, generalized Whittle–Matérn fields on manifolds or surfaces can be considered in future work. This extension is of relevance for practical applications in statistics, where for instance models on the sphere often play an important role. In fact, for a smooth surface  $\mathcal{M}$  without boundary, such as the sphere, the transition from the abstract results of Section 2 to Whittle–Matérn fields on  $\mathcal{M}$  should be more straightforward compared to the arguments used in Section 4 for bounded Euclidean domains. This is suggested by the fact that on a smooth surface  $\mathcal{M}$  (and for smooth coefficients  $\mathbf{a}, \kappa$ ) the space  $\dot{H}_L^r$  is isomorphic to the Sobolev space  $H^r(\mathcal{M})$ , and not to a proper subspace thereof (4.7) containing only functions which satisfy certain boundary conditions.

## Acknowledgements

The authors thank the editor and the reviewers for their valuable comments which led to an improved, more accessible presentation of the results.

## Supplementary Material

**Supplement to “Equivalence of measures and asymptotically optimal linear prediction for Gaussian random fields with fractional-order covariance operators”** (DOI: [10.3150/22-BEJ1507SUPP](https://doi.org/10.3150/22-BEJ1507SUPP); .pdf). The supplementary material contains the six appendices A, B, C, D, E, and F with auxiliary results and proofs.

## References

- [1] Adams, R.A. and Fournier, J.J.F. (2003). *Sobolev Spaces*, 2nd ed. *Pure and Applied Mathematics (Amsterdam)* **140**. Amsterdam: Elsevier/Academic Press. [MR2424078](#)
- [2] Anderes, E. (2010). On the consistent separation of scale and variance for Gaussian random fields. *Ann. Statist.* **38** 870–893. [MR2604700](#) <https://doi.org/10.1214/09-AOS725>
- [3] Andreev, R. (2016). ppfem – MATLAB routines for the FEM with piecewise polynomial splines on product meshes. Available at <https://bitbucket.org/numpde/ppfem/>, retrieved on November 11, 2017.
- [4] Bakka, H., Vanhatalo, J., Illian, J.B., Simpson, D. and Rue, H. (2019). Non-stationary Gaussian models with physical barriers. *Spat. Stat.* **29** 268–288. [MR3903698](#) <https://doi.org/10.1016/j.spasta.2019.01.002>
- [5] Bogachev, V.I. (1998). *Gaussian Measures. Mathematical Surveys and Monographs* **62**. Providence, RI: Amer. Math. Soc. [MR1642391](#) <https://doi.org/10.1090/surv/062>
- [6] Bolin, D., Kirchner, K. (2023). Supplement to “Equivalence of measures and asymptotically optimal linear prediction for Gaussian random fields with fractional-order covariance operators.” <https://doi.org/10.3150/22-BEJ1507SUPP>
- [7] Bolin, D. and Kirchner, K. (2020). The rational SPDE approach for Gaussian random fields with general smoothness. *J. Comput. Graph. Statist.* **29** 274–285. [MR4116041](#) <https://doi.org/10.1080/10618600.2019.1665537>
- [8] Bolin, D., Kirchner, K. and Kovács, M. (2018). Weak convergence of Galerkin approximations for fractional elliptic stochastic PDEs with spatial white noise. *BIT* **58** 881–906. [MR3882975](#) <https://doi.org/10.1007/s10543-018-0719-8>
- [9] Bolin, D., Kirchner, K. and Kovács, M. (2020). Numerical solution of fractional elliptic stochastic PDEs with spatial white noise. *IMA J. Numer. Anal.* **40** 1051–1073. [MR4092278](#) <https://doi.org/10.1093/imanum/dry091>
- [10] Bolin, D. and Lindgren, F. (2011). Spatial models generated by nested stochastic partial differential equations, with an application to global ozone mapping. *Ann. Appl. Stat.* **5** 523–550. [MR2810408](#) <https://doi.org/10.1214/10-AOAS383>
- [11] Borovitskiy, V., Terenin, A., Mostowsky, P. and Deisenroth, M.P. (2020). Matérn Gaussian processes on Riemannian manifolds. In *Advances in Neural Information Processing Systems* **33** 12426–12437. Curran Associates.
- [12] Cox, S.G. and Kirchner, K. (2020). Regularity and convergence analysis in Sobolev and Hölder spaces for generalized Whittle-Matérn fields. *Numer. Math.* **146** 819–873. [MR4182088](#) <https://doi.org/10.1007/s00211-020-01151-x>
- [13] Da Prato, G. and Zabczyk, J. (2014). *Stochastic Equations in Infinite Dimensions*, 2nd ed. *Encyclopedia of Mathematics and Its Applications* **152**. Cambridge: Cambridge Univ. Press. [MR3236753](#) <https://doi.org/10.1017/CBO9781107295513>
- [14] Davies, E.B. (1995). *Spectral Theory and Differential Operators. Cambridge Studies in Advanced Mathematics* **42**. Cambridge: Cambridge Univ. Press. [MR1349825](#) <https://doi.org/10.1017/CBO9780511623721>
- [15] Dunford, N. and Schwartz, J.T. (1963). *Linear Operators. Part II: Spectral Theory. Self Adjoint Operators in Hilbert Space*. New York: Interscience Publishers Wiley. With the assistance of William G. Bade and Robert G. Bartle. [MR0188745](#)
- [16] Fuglstad, G.-A., Simpson, D., Lindgren, F. and Rue, H. (2015). Does non-stationary spatial data always require non-stationary random fields? *Spat. Stat.* **14** 505–531. [MR3431054](#) <https://doi.org/10.1016/j.spasta.2015.10.001>
- [17] Grisvard, P. (1967). Caractérisation de quelques espaces d’interpolation. *Arch. Ration. Mech. Anal.* **25** 40–63. [MR0213864](#) <https://doi.org/10.1007/BF00281421>
- [18] Guinness, J. and Fuentes, M. (2016). Isotropic covariance functions on spheres: Some properties and modeling considerations. *J. Multivariate Anal.* **143** 143–152. [MR3431424](#) <https://doi.org/10.1016/j.jmva.2015.08.018>
- [19] Guttorp, P. and Gneiting, T. (2006). Studies in the history of probability and statistics. XLIX. On the Matérn correlation family. *Biometrika* **93** 989–995. [MR2285084](#) <https://doi.org/10.1093/biomet/93.4.989>
- [20] Herrmann, L., Kirchner, K. and Schwab, C. (2020). Multilevel approximation of Gaussian random fields: Fast simulation. *Math. Models Methods Appl. Sci.* **30** 181–223. [MR4059369](#) <https://doi.org/10.1142/s0218202520500050>

- [21] Hildeman, A., Bolin, D. and Rychlik, I. (2021). Deformed SPDE models with an application to spatial modeling of significant wave height. *Spat. Stat.* **42** Paper No. 100449. [MR4233262](#) <https://doi.org/10.1016/j.spasta.2020.100449>
- [22] Kirchner, K. and Bolin, D. (2022). Necessary and sufficient conditions for asymptotically optimal linear prediction of random fields on compact metric spaces. *Ann. Statist.* **50** 1038–1065. [MR4404928](#) <https://doi.org/10.1214/21-aos2138>
- [23] Lindgren, F., Rue, H. and Lindström, J. (2011). An explicit link between Gaussian fields and Gaussian Markov random fields: The stochastic partial differential equation approach. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **73** 423–498. With discussion and a reply by the authors. [MR2853727](#) <https://doi.org/10.1111/j.1467-9868.2011.00777.x>
- [24] Lions, J.-L. and Magenes, E. (1972). *Non-homogeneous Boundary Value Problems and Applications. Vol. I. Die Grundlehren der Mathematischen Wissenschaften, Band 181*. New York: Springer. [MR0350177](#)
- [25] Lunardi, A. (2018). *Interpolation Theory. Appunti. Scuola Normale Superiore di Pisa (Nuova Serie) [Lecture Notes. Scuola Normale Superiore di Pisa (New Series)]* **16**. Pisa: Edizioni della Normale. [MR3753604](#) <https://doi.org/10.1007/978-88-7642-638-4>
- [26] Matérn, B. (1960). *Spatial Variation: Stochastic Models and Their Application to Some Problems in Forest Surveys and Other Sampling Investigations*. Stockholm: Statens Skogsforskningsinstitut. Meddelanden Från Statens Skogsforskningsinstitut, Band 49, Nr. 5. [MR0169346](#)
- [27] Rasmussen, C.E. and Williams, C.K.I. (2006). *Gaussian Processes for Machine Learning. Adaptive Computation and Machine Learning*. Cambridge, MA: MIT Press. [MR2514435](#)
- [28] Stein, M.L. (1993). A simple condition for asymptotic optimality of linear predictions of random fields. *Statist. Probab. Lett.* **17** 399–404. [MR1237787](#) [https://doi.org/10.1016/0167-7152\(93\)90261-G](https://doi.org/10.1016/0167-7152(93)90261-G)
- [29] Stein, M.L. (1997). Efficiency of linear predictors for periodic processes using an incorrect covariance function. *J. Statist. Plann. Inference* **58** 321–331. [MR1450019](#) [https://doi.org/10.1016/S0378-3758\(96\)00088-2](https://doi.org/10.1016/S0378-3758(96)00088-2)
- [30] Stein, M.L. (1999). *Interpolation of Spatial Data: Some Theory for Kriging. Springer Series in Statistics*. New York: Springer. [MR1697409](#) <https://doi.org/10.1007/978-1-4612-1494-6>
- [31] Thomée, V. (2006). *Galerkin Finite Element Methods for Parabolic Problems*, 2nd ed. *Springer Series in Computational Mathematics* **25**. Berlin: Springer. [MR2249024](#)
- [32] Triebel, H. (1978). *Interpolation Theory, Function Spaces, Differential Operators. North-Holland Mathematical Library* **18**. Amsterdam: North-Holland. [MR0503903](#)
- [33] Whittle, P. (1963). Stochastic processes in several dimensions. *Bull. Inst. Internat. Statist.* **40** 974–994. [MR0173287](#)
- [34] Zhang, H. (2004). Inconsistent estimation and asymptotically equal interpolations in model-based geostatistics. *J. Amer. Statist. Assoc.* **99** 250–261. [MR2054303](#) <https://doi.org/10.1198/016214504000000241>

Received September 2021 and revised February 2022