# Highlights

## **Optimal Sampling Density for Nonparametric Regression**

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- We derive a novel *active learning* framework, based on the *local polynomial smoothing* model class
- It samples from the *optimal training density* that asymptotically minimizes the generalization error of *local polynomial smoothing*
- The *optimal training density* is *interpretable* as it factorizes the influence of local, problem intrinsic properties such as the *noise level, function complexity* and *test relevance*
- We apply local bandwidth estimates via *Lepski's method* to provide an implementation of our *active learning* framework in the *isotropic* case
- We provide empirical evidence that our proposed *active learning* framework is *model-agnostic* by applying it to a neural network and a random forest model

## Optimal Sampling Density for Nonparametric Regression

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## Abstract

We propose a novel active learning strategy for regression, which is modelagnostic, robust against model mismatch, and interpretable. Assuming that a small number of initial samples are available, we derive the optimal training density that minimizes the generalization error of local polynomial smoothing (LPS) with its kernel bandwidth tuned locally: We adopt the *mean integrated* squared error (MISE) as a generalization criterion, and use the asymptotic behavior of the MISE as well as the locally optimal bandwidths (LOB) – the bandwidth function that minimizes MISE in the asymptotic limit. The asymptotic expression of our objective then reveals the dependence of the MISE on the training density, enabling analytic minimization. As a result, we obtain the optimal training density in a closed-form. The almost modelfree nature of our approach thus helps to encode the essential properties of the target problem, providing a robust and model-agnostic active learning strategy. Furthermore, the obtained training density factorizes the influence of local function complexity, noise level and test density in a transparent and interpretable way. We validate our theory in numerical simulations, and show that the proposed active learning method outperforms the existing state-of-the-art model-agnostic approaches.

*Keywords:* Adaptive kernel bandwidth, Lepski's method, local polynomial smoothing, local function complexity, active learning

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#### 1. Introduction

Active learning is a powerful tool for inference when acquiring labels is expensive. Given a fixed budget of labels that may be queried, the basic idea is to construct a training set in a way that minimizes a predefined generalization loss. Active learning for classification has been applied successfully in learning approaches to text categorization (Lewis and Gale, 1994; Roy and McCallum, 2001; Goudjil et al., 2018), biomedical data analysis (Warmuth et al., 2003; Pasolli and Melgani, 2010; Saito et al., 2015; Bressan et al., 2019), image classification (Sener and Savarese, 2018; Beluch et al., 2018; Haut et al., 2018) and image retrieval (Tong and Chang, 2001; He, 2010). In the classification regime these approaches were able to reduce the required amount of training data drastically, where the selection criteria are commonly based on input space geometric arguments. For example, one may request labels close to the decision boundary, for which the prediction uncertainty is high (Tong and Chang, 2001; Warmuth et al., 2003). This way, most of the input space that is associated to the interior of the class supports can be neglected while training. More recently, active learning was deployed in regression tasks such as wind speed forecasting (Douak et al., 2013), optimal control (Wu et al., 2020) and reinforcement learning (Teytaud et al., 2007), quantum chemistry (Tang and de Jong, 2019; Gubaev et al., 2018) and industrial applications in semiconductor manufacturing (Sugiyama and Nakajima, 2009).

Active learning approaches can be categorized with respect to several properties such as informativeness, representativeness and diversity (Settles, 2010; Wu, 2019) and we refer to the broad overview of literature on active learning reviewed by Settles (2010). Each active learning approach induces a sampling scheme, by which we mean the process of successively adding new labeled instances to the training dataset. In this paper we distinguish between supervised and unsupervised sampling schemes: A supervised sampling scheme is based on a sampling criterion that depends on the so far acquired training labels. Any sampling scheme that is not *supervised* is hence regarded as unsupervised. We will refer to i.i.d. sampling from some test distribution as random test sampling, which is the most simple unsupervised baseline. Note that in the literature of active learning the notion of unsupervised sampling schemes (Liu et al., 2021) are synonymously referred to as *passive* (Yu and Kim, 2010; Wu, 2019) or blind (Teytaud et al., 2007). Furthermore, we will call a sampling scheme *model-based*, if the derivation of its sampling criterion involves a model of the function to infer. Whether this particular model is *parametric* or *nonparametric*, it is furthermore reasonable to differentiate between a parametric or nonparametric sampling scheme. In contrast, we

regard any sampling scheme that is not model-based as model-free.

**Remark 1.** The two properties, whether a sampling scheme is (un)supervised or model-based/free, are complementary in the sense that we find sampling schemes with an arbitrary combination of characteristics of these properties.

We will now address those aspects that are relevant to classify our algorithmic proposal of a novel active learning framework for regression. Clearly, every category has its share of the domain of learning problems where it performs best (see Sec. 4.3 for further in-depth discussion).

Properties of sampling schemes: We call a sampling scheme

- **optimal**, if it optimizes some risk with respect to a prediction model that is deployed on the learning task.
- **robust**, if its sampling criterion imposes at most mild assumptions on the regularity of the labels.
- model-agnostic, if the performance of an arbitrary, but reasonable model with the acquired training set is not worse (ideally better) than using a random test sample.

An *optimal* sampling scheme allows for the maximal performance gain, as long as we can fix the final prediction model in advance. Note that the *optimal* sampling scheme may strongly depend on the prediction model.

In real-world scenarios we often face the situation that domain knowledge is scarce, and thus we are not aware about the regularity of the problem and committing to a final model might be premature. This means that practitioners will prefer a consistent, yet moderate performance increase provided by a *robust* sampling scheme rather than risking to have overestimated the regularity of the problem that an *optimal* sampling scheme may assume. Under violation of such assumptions, the quality of the so acquired training set may deteriorate below *random test sampling*. On the other hand, the state-of-the-art for such a scenario is rapidly evolving and so, as also noted by Settles (2010), it is advantageous if an acquired training set remains meaningful after model adaption. In this regard, it is desirable for a sampling scheme to be *model-agnostic*.

In this work, our goal is to find a sampling scheme that is simultaneously *optimal*, *robust* and *model-agnostic*. As we will discuss in Sec. 4.1, such a sampling scheme must necessarily be supervised and nonparametric. We will base our active learning framework on *local polynomial smoothing* (LPS) (see, for example, Cleveland and Devlin (1988)), a nonparametric model class with

minimal regularity assumptions on the labels. We consider LPS as almost model-free.

We will now outline our main contribution. Intuitively, we consider the best achievable MISE within the LPS model class as our objective which we then aim to minimize with respect to the training distribution. Ultimately, our active learning strategy is to sample from this training distribution.

Let f be the target regression function that we want to infer from noisy observations  $y_i = f(x_i) + \varepsilon_i$ , where  $\varepsilon_i$  is independently drawn from a distribution with mean  $\mathbb{E}[\varepsilon_i] = 0$  and local noise variance  $\mathbb{V}[\varepsilon_i] = v(x_i)$ , and  $x_i \sim p$  are i.i.d. samples according to a training probability density p defined on  $\mathcal{X} \subset \mathbb{R}^d$ . Furthermore let  $k^{\Sigma}(x, x') := |\Sigma|^{-1} k(||\Sigma^{-1}(x - x')||)$  be a radial basis function (RBF) kernel, where the positive definite bandwidth matrix parameter  $\Sigma \in \mathbb{S}^d_{++}$  controls the degree of localization. Here, we denote by |M| the determinant of the square matrix  $M \in \mathbb{R}^{d \times d}$ .

Let  $\mathcal{P}_Q(\mathbb{R}^d)$  be the space of the real polynomial mappings  $\mathfrak{p} \colon \mathbb{R}^d \to \mathbb{R}$ up to order Q. For a training set  $\mathbf{X}_n = \{x_i\}_{i=1}^n \in \mathcal{X}^n$  of size n, the LPS predictor of order Q is given by

$$m_Q^{\Sigma}(x) = \mathfrak{p}_{Q,\Sigma,x}^*(0), \text{ where}$$

$$\mathfrak{p}_{Q,\Sigma,x}^* = \operatorname*{arg\,min}_{\mathfrak{p}\in\mathcal{P}_Q(\mathbb{R}^d)} \sum_{i=1}^n k^{\Sigma}(x_i, x) \left(y_i - \mathfrak{p}(x_i - x)\right)^2.$$

$$(1)$$

Here,  $\mathfrak{p}_{Q,\Sigma,x}^*$  is the optimal local polynomial approximation of f around x. In particular,  $\mathfrak{p}_{Q,\Sigma,x}^*(0)$  gives the approximate function value at x.

The simplicity of the LPS formulation allows for rich analysis as amongst others demonstrated by Fan and Gijbels (1992); Ruppert and Wand (1994) in the special case of *local linear smoothing* (LLS), where Q = 1, and in the general case by Fan et al. (1997); Masry (1996, 1997). Let  $S \subseteq \mathbb{S}_{++}^d$  be a candidates set of positive definite bandwidth matrices. Since the prediction (1) of LPS involves solving an individual problem for each test point  $x \in \mathcal{X}$ , the bandwidth  $\Sigma \in S$  can be chosen individually in x without affecting the prediction of any other instance  $x' \neq x$ . Thus, given a training set  $X_n$  and a performance measure such as the *conditional mean squared error* 

$$MSE_Q(x, \Sigma | \boldsymbol{X}_n) = \mathbb{E}\left[ (m_Q^{\Sigma}(x) - f(x))^2 | \boldsymbol{X}_n \right],$$

we are free to tune  $\Sigma_x \in \mathcal{S}$  in x such that, ideally,

$$MSE_Q(x, \Sigma_x | \mathbf{X}_n) = \inf_{\Sigma \in \mathcal{S}} MSE_Q(x, \Sigma | \mathbf{X}_n).$$
(2)

Our criterion for optimization of  $X_n$  is then as follows: Given a test density q on  $\mathcal{X}$  and a training set  $X_n$ , we may define the optimal *mean integrated* squared error by

$$\operatorname{MISE}_{Q}\left(q|\boldsymbol{X}_{n}\right) = \int_{\mathcal{X}} \operatorname{inf}_{\Sigma \in \mathcal{S}} \operatorname{MSE}_{Q}\left(x, \Sigma | \boldsymbol{X}_{n}\right) q(x) dx.$$
(3)

Note that the infimum over  $\Sigma \in S$  is taken for each x before integration over x. As our ultimate goal, we therefore seek to tune the training set choice  $X_n^*$  such that

$$\boldsymbol{X}_{n}^{*} \approx \inf_{\boldsymbol{X}_{n} \in \mathcal{X}^{n}} \operatorname{MISE}_{Q}\left(q | \boldsymbol{X}_{n}\right).$$

$$\tag{4}$$

The main idea of our theory is to express the objective (3) asymptotically as a function of the training density p, the local noise level v, the training size n, the test density q and a measure of *local function complexity* (LFC) that concentrates local information about f into a scalar value in a natural way. Since the dependence of the MISE on p is given explicitly in the form we will derive, we will be able to analytically optimize our objective (3) with respect to the training density. In other words, we will obtain a training density  $p_{\text{Opt}}^{Q,n}$ that is asymptotically optimal, and our proposed active learning approach samples training data  $X_n^* \sim p_{\text{Opt}}^{Q,n}$ . As we will demonstrate in Sec. 4.2, this sampling scheme encompasses all desired properties. That is, it is *optimal*, *robust* and *model-agnostic*. Additionally it turns out to be *stationary* and *interpretable* as well – two properties, we will also define and discuss in Sec. 4. While stationarity enables batch sampling in a natural way, interpretability gives access to a representation of the sampling scheme that is comprehensible by humans.

In order to be able to express the objective (3) in this manner, a fundamental step is to guarantee the existence and understand the asymptotics of  $\Sigma_x$  in the sense of (2). We will refer to  $\Sigma_x$  as a locally optimal bandwidth (LOB) in  $x \in \mathcal{X}$  in the following. In case of the isotropic bandwidth candidate set  $S = \{\sigma \mathcal{I}_d \mid \sigma > 0\}$ ,  $\Sigma_x$  is unique, and there exist known results on its asymptotic behavior (Fan and Gijbels, 1992; Ruppert and Wand, 1994; Fan et al., 1997; Masry, 1996, 1997) as well as its estimation (Zhang and Chan, 2011).

When considering a non-isotropic bandwidth candidate set instead,  $\Sigma_x$  will typically not be unique, and its asymptotics behaves differently. Accordingly, care needs to be taken when trying to generalize the results from the isotropic to the non-isotropic case. We provide first results for an extension of our theory to the non-isotropic case in Appendix B. Yet, as we require an estimate of general, positive definite LOB in practice – which is currently an open research question for the non-isotropic case – we are only able to give an initial theory to the non-isotropic case in Appendix B; this theory will immediately become applicable once an estimate to non-isotropic LOB will come to existence. In the remainder of this work, we therefore focus on the isotropic case.

We will begin with an introduction into previous research, followed by the derivation of our main theorem in Sec. 2. We provide implementation details in Sec. 3 and discuss active learning properties and related work in Sec. 4. Then we demonstrate the capabilities of our proposed framework in experiments on toy-data in Sec. 5: We show its benefits in settings of inhomogeneous complexity and heteroscedasticity and compare favorably to two related nonparametric active learning approaches that were built to work on the respective dataset. Finally, we conclude in Sec. 6.

#### 2. Analyzing Optimal Training in the Isotropic Case

In the following, we denote by  $vec(S) \in \mathbb{R}^N$  the arbitrarily, but fixed ordered vectorization of a finite set S of cardinality N = |S|. While for our purpose the order of this vectorization does not matter, it should be applied consistently. For  $A \subset \mathbb{R}^a, B \subset \mathbb{R}^b$  and  $c \ge 0$  let  $\mathcal{C}^c(A, B)$  be the set of c-times continuously differentiable functions  $f: A \to B$ . As a shorthand let  $\mathcal{C}^c(A) := \mathcal{C}^c(A, \mathbb{R})$ . For  $f \in \mathcal{C}^c(A, B)$  and  $l \le c$  let  $D_f^l(x)$  the tensor of l-th order partial derivatives of f in  $x \in A$ . Finally, we denote by  $X_n = o_p[a_n]$ the convergence in probability of a random sequence  $X_n$ , meaning that for all  $\varepsilon > 0$  it is  $\mathbb{P}(|X_n/a_n| \ge \varepsilon) \to 0$  as  $n \to \infty$ , and by  $X_n = O_p[a_n]$  the stochastic boundedness, meaning that for all  $\varepsilon > 0$  there exists M > 0 and  $N \in \mathbb{N}$  such that  $\mathbb{P}(|X_n/a_n| > M) < \varepsilon, \forall n > N$ . A list of frequently used abbreviations and mathematical symbols can be found in Appendix A.

If  $\Sigma_x$  in (2) uniquely exists for all x, such that for all  $\Sigma \in \mathcal{S}$  with  $\Sigma \neq \Sigma_x$ it is  $\text{MSE}_Q(x, \Sigma_x | \mathbf{X}_n) < \text{MSE}_Q(x, \Sigma | \mathbf{X}_n)$ , we can define the *locally optimal* bandwidth function (LOB) as

$$\Sigma_Q^n(x) = \operatorname{argmin}_{\Sigma \in \mathcal{S}} \operatorname{MSE}_Q(x, \Sigma | \boldsymbol{X}_n).$$
(5)

In this case, we are also able to define the oracle local kernel regressor by

$$\hat{f}_{\text{Opt}}^Q(x) = m_Q^{\Sigma_Q^0(x)}(x).$$
(6)

**Remark 2.** For any regression model  $\hat{f}$  we can define the MISE as

$$MISE\left(q, \widehat{f} | \boldsymbol{X}_n\right) = \int_{\mathcal{X}} \mathbb{E}\left[(\widehat{f}(x) - f(x))^2 | \boldsymbol{X}_n\right] q(x) dx.$$

Accordingly, we can write  $MISE_Q(q|\boldsymbol{X}_n) = MISE\left(q, \hat{f}_{Opt}^Q|\boldsymbol{X}_n\right).$ 

There are known results that guarantee LOB in (5) to be well-defined, which means that the minimizer exists and is unique: We refer, for example, to the work of Masry (1996, 1997) in the case of isotropic bandwidth candidates  $S = \{\sigma \mathcal{I}_d \mid \sigma > 0\}$ , and to Fan et al. (1997) in the general case  $S = \mathbb{S}_{++}^d$  for Q = 1. All these results rely on the antagonizing effect of bias and variance: Generally, we can decompose the conditional MSE in  $x \in \mathcal{X}$  (see Geman et al. (1992); Bishop (2006)) according to

$$MSE_Q(x, \Sigma | \boldsymbol{X}_n) = \mathbb{B}_Q(x, \Sigma | \boldsymbol{X}_n)^2 + \mathbb{V}_Q(x, \Sigma | \boldsymbol{X}_n), \quad \text{where} \quad (7)$$
$$\mathbb{B}_Q(x, \Sigma | \boldsymbol{X}_n) = f(x) - \mathbb{E}\left[m_Q^{\Sigma}(x) | \boldsymbol{X}_n\right] \quad \text{and}$$
$$\mathbb{V}_Q(x, \Sigma | \boldsymbol{X}_n) = \mathbb{E}\left[(m_Q^{\Sigma}(x) - \mathbb{E} m_Q^{\Sigma}(x))^2 | \boldsymbol{X}_n\right]$$

are the bias- and variance-related error terms. Now, as  $\|\Sigma\| \to 0$ ,  $\mathbb{B}_Q(x, \Sigma | \mathbf{X}_n)$  decreases while  $\mathbb{V}_Q(x, \Sigma | \mathbf{X}_n)$  increases; On the other hand, as  $|\Sigma| \to \infty$ ,  $\mathbb{B}_Q(x, \Sigma | \mathbf{X}_n)$  increases while  $\mathbb{V}_Q(x, \Sigma | \mathbf{X}_n)$  decreases. It is known that there is a finite bandwidth that trades off both terms in the optimal way (Silverman, 1986; Wand and Jones, 1994). After identifying the leading terms of bias and variance, an asymptotic closed-form solution to  $\Sigma_Q^n$  can be constructed explicitly in the isotropic case for arbitrary.

In this paper, we will focus on the case where the bandwidth space is restricted to be isotropic. In this case, we can elaborate our framework from the theoretical point-of-view by making use of the results of Masry (1996, 1997) on the unique existence and asymptotic behavior of LOB under mild assumptions. Furthermore, we can estimate LOB (Zhang and Chan, 2011) by Lepski's method (Lepski, 1991; Lepski and Spokoiny, 1997).

The approach of using the asymptotic closed-form solution to LOB to prove our theory however cannot be generalized to the non-isotropic case without imposing unrealistically strong assumptions. We will discuss these issues that do arise in the non-isotropic bandwidth case – when in particular not relying on this explicit construction – and provide solutions that still make our theory hold under mild conditions in Appendix B.

#### 2.1. Preliminaries

Let us begin by making the LPS predictor from (1) explicit: Define the vector of distinct *j*-th order monomials of  $u \in \mathbb{R}^d$  by

$$m_{j}(u) = \operatorname{vec}\left(\left\{\prod_{l=1}^{d} u_{l}^{j_{l}} \mid \boldsymbol{j} : \sum_{k=1}^{d} \boldsymbol{j}_{k} = \boldsymbol{j}\right\}\right).$$

$$(8)$$

Note that  $m_j(u) \in \mathbb{R}^{N_j}$  for  $N_j = \binom{d-1+j}{d-1}$ . Now, we can write any polynomial  $\mathfrak{p} \in \mathcal{P}_Q(\mathbb{R}^d)$  of order Q as  $\mathfrak{p}(z) = \sum_{j=0}^Q \beta_j^\top m_j(z)$ , where the mapping between  $\mathfrak{p}$  and its monomial coefficients  $\beta_j \in \mathbb{R}^{N_j}$  is bijective. For convenience, we will identify a polynomial with its coefficients and use both expressions interchangeably. In this regard, let  $(\beta_{Q,x}^{\Sigma})_0^*, \ldots, (\beta_{Q,x}^{\Sigma})_Q^*$  be the coefficients of the optimal polynomial  $\mathfrak{p}_{Q,\Sigma,x}^*$ . Noting that  $\mathfrak{p}(0) = \beta_0 \in \mathbb{R}$ , the optimization in (1) is expressed as

$$m_Q^{\Sigma}(x) = \left(\beta_{Q,x}^{\Sigma}\right)_0^*, \text{ where}$$
(9)

$$\left(\beta_{Q,x}^{\Sigma}\right)_{0}^{*},\ldots,\left(\beta_{Q,x}^{\Sigma}\right)_{Q}^{*}=\operatorname*{argmin}_{\beta_{0},\ldots,\beta_{Q}}\sum_{i=1}^{n}k^{\Sigma}(x_{i},x)\left[y_{i}-\sum_{j=0}^{Q}\beta_{j}^{\top}m_{j}(x_{i}-x)\right]^{2}$$

Let us aggregate the vector of distinct monomials up to order Q as

$$M_Q(u) = [m_0(u)^{\top}, \dots, m_Q(u)^{\top}]^{\top}.$$
 (10)

The following closed-form solution for (9) is known (see, for example, Zhang and Chan (2011)): Letting  $X_Q(x) = [M_Q(x_1 - x), \dots, M_Q(x_n - x)]^\top$  and  $W_x^{\Sigma} = diag([k^{\Sigma}(x_1, x), \dots, k^{\Sigma}(x_n, x)])$ , it is

$$\begin{split} m_Q^{\Sigma}(x) &= A_Q^{\Sigma}(x) Y_n, \text{ where} \\ A_Q^{\Sigma}(x) &= e_1^{\top} \left( X_Q(x)^{\top} W_x^{\Sigma} X_Q(x) \right)^{-1} X_Q(x)^{\top} W_x^{\Sigma}. \end{split}$$

By substituting the equation above into Eq. (7), we obtain

$$MSE_Q(x, \Sigma | \boldsymbol{X}_n) = \mathbb{B}_Q(x, \Sigma | \boldsymbol{X}_n)^2 + \mathbb{V}_Q(x, \Sigma | \boldsymbol{X}_n), \quad \text{where}$$

$$\mathbb{B}_Q(x, \Sigma | \boldsymbol{X}_n) = f(x) - A_Q^2(x) f(\boldsymbol{X}_n) \quad \text{and} \quad (11)$$

$$\mathbb{V}_Q(x, \Sigma | \boldsymbol{X}_n) = A_Q^{\Sigma}(x) \boldsymbol{diag}(v(\boldsymbol{X}_n)) A_Q^{\Sigma}(x)^{\top}.$$
(12)

From here on, we assume for simplicity that the input space  $\mathcal{X} \subset \mathbb{R}^d$  is compact, which real-world data will typically fulfill<sup>1</sup>. As mentioned above,

<sup>&</sup>lt;sup>1</sup>The theory may be extended to more general cases by imposing a weaker condition than compactness, such as bounded derivatives and a fast enough decay of the kernel.

we restrict ourselves to the case of isotropic bandwidth candidates  $S = \{\sigma I_d \mid \sigma > 0\}$ . Under adequate regularity conditions, explicit asymptotic formulations for LOB are known (see, for example, Fan and Gijbels (1992); Fan et al. (1997) and Masry (1996, 1997)): Using (10), define by

$$\boldsymbol{M}_{Q} = \int_{\mathcal{X}} M_{Q}(\boldsymbol{u}) M_{Q}(\boldsymbol{u})^{\top} \boldsymbol{k}(\boldsymbol{u}) d\boldsymbol{u}, \quad \text{and} \quad \boldsymbol{\Gamma}_{Q} = \int_{\mathcal{X}} M_{Q}(\boldsymbol{u}) M_{Q}(\boldsymbol{u})^{\top} \boldsymbol{k}^{2}(\boldsymbol{u}) d\boldsymbol{u}$$

the first and second moment matrix of the kernel, by

$$\boldsymbol{D}_Q(x) = \left\{ \left[ \prod_{k=1}^d \boldsymbol{j}_k! \right]^{-1} \frac{\partial^{Q+1}}{\prod_{l=1}^d \partial^{\boldsymbol{j}_l} x_l} f(x) \; \middle| \; \boldsymbol{j} : \sum_{k=1}^d \boldsymbol{j}_k = Q+1 \right\},$$

the vector of distinct partial derivatives of f of order Q + 1 in x, and

$$\boldsymbol{B}_Q = \int_{\mathcal{X}} M_Q(\boldsymbol{u}) \boldsymbol{m}_{Q+1}(\boldsymbol{u})^\top \boldsymbol{k}(\boldsymbol{u}) d\boldsymbol{u}.$$

**Theorem 3** (Masry (1996, 1997)). Let  $k^{\Sigma}(x, x') = |\Sigma|^{-1} k(\Sigma^{-1}(x - x'))$  be a not necessarily spherically symmetric kernel. Let  $h_n \to 0$ ,  $nh_n^d \to \infty$  as  $n \to \infty$  and x be a fixed point in the interior of  $\{x \mid p(x) > 0\}$ . Furthermore let  $f \in C^{Q+1}(\mathcal{X}), p \in C^1(\mathcal{X})$  and  $v \in C^0(\mathcal{X})$  with  $\inf_{x \in \mathcal{X}} p(x) > 0$  and  $\inf_{x \in \mathcal{X}} v(x) > 0$ . The bias and variance of LPS of order Q can asymptotically be expressed as

$$\mathbb{B}_{Q}\left(x,h_{n}\mathcal{I}_{d}|\boldsymbol{X}_{n}\right) = bias_{Q}\left[x,h_{n}\mathcal{I}_{d}\right] + o_{p}\left[h_{n}^{Q+1}\right]$$

and

$$\mathbb{V}_{Q}\left(x, h_{n}\mathcal{I}_{d} | \boldsymbol{X}_{n}\right) = var_{Q}\left[x, h_{n}\mathcal{I}_{d} | \boldsymbol{X}_{n}\right] + o_{p}\left[n^{-1}h_{n}^{-d}\right]$$

where

$$bias_Q[x, h_n \mathcal{I}_d] = h_n^{Q+1} e_1^\top \boldsymbol{M}_Q^{-1} \boldsymbol{B}_Q \boldsymbol{D}_Q(x)$$
(13)

is the leading bias-term of order Q+1, and for  $\mathbf{R}_Q = e_1^\top \mathbf{M}_Q^{-1} \mathbf{\Gamma}_Q \mathbf{M}_Q^{-1} e_1$ ,

$$var_Q\left[x, h_n \mathcal{I}_d | \boldsymbol{X}_n\right] = \boldsymbol{R}_Q \frac{v(x)}{p(x)nh_n^d}.$$
(14)

In Theorem 3 and in the following, we call the kernel k spherically symmetric, if its evaluation in  $x \in \mathcal{X}$  only depends on x through its norm ||x||. That is, we can rewrite  $k(x) = \tilde{k}(||x||)$  for some adequate function  $\tilde{k}$ .

**Remark 4.** If the kernel k is spherically symmetric and Q is even, then  $bias_Q[x, h_n \mathcal{I}_d] = 0$  and  $var_Q[x, h_n \mathcal{I}_d | \mathbf{X}_n] = var_{Q+1}[x, h_n \mathcal{I}_d | \mathbf{X}_n]$ , since  $\mathbf{R}_Q = \mathbf{R}_{Q+1}$ . In this case, if  $f \in C^{Q+2}(\mathcal{X})$ , the leading bias term will be of the form  $b_Q(x, h_n \mathcal{I}_d) = bias_{Q+1}[x, h_n \mathcal{I}_d] + O_p[h_n^{Q+2}]$ . Here, it is common belief that  $b_Q(x, h_n \mathcal{I}_d) > bias_{Q+1}[x, h_n \mathcal{I}_d]$  (see, for example, Fan et al. (1997)). Thus, as we have to require  $f \in C^{Q+2}(\mathcal{X})$  anyhow, and the variance does not grow when moving from the LPS model of order Q to Q + 1, we expect a better performance when using the LPS model of (odd) order Q + 1. Note that the performance increases only by a constant factor and not in convergence rate, when applying LPS of order Q + 1 instead of Q. More importantly in the context of our work, the LPS model of odd order Q + 1 is design-adaptive (Fan, 1992). That is, the leading bias-term  $bias_{Q+1}[x, h_n \mathcal{I}_d]$ does not depend on the derivatives of the training distribution. In contrast, for example, the bias of the Nadaraya-Watson estimator (LPS of order Q = 0) is

$$b_0(x, h_n \mathcal{I}_d) = bias_1[x, h_n \mathcal{I}_d] + h_n^2 \mu_2 \frac{1}{p(x)} \sum_{i=1}^d \frac{\partial f}{\partial x_i}(x) \frac{\partial p}{\partial x_i}(x),$$

where  $\mu_2 = \int u^2 k(u) du$ . Here, the bias obviously depends on the derivative of p. In this case, as also noted by Fan (1992), the model has problems to adapt to highly clustered distributions, where  $\left|\frac{1}{p(x)}\frac{\partial p}{\partial x_i}(x)\right|$  is large.

**Remark 5.** Note that we could also use a kernel of higher order  $\nu > 2$  to adapt optimally to functions of higher smoothness  $f \in C^{\nu}(\mathcal{X})$  without the need to increase the polynomial order Q of LPS. However, a higher-order kernel loses consistency as it necessarily takes negative values (Györfi et al., 2002), and it loses design-adaptivity for  $Q < \nu - 1$ .

In the upcoming derivation of our theory, we rely on design-adaptivity to keep the optimization of the conditional MSE with respect to the training distribution simple. Design-adaptivity is guaranteed, if the leading order bias term (13) does not vanish. In the light of Remark 4, it is reasonable to choose a spherically symmetric kernel for odd order Q. For even order Q, for example, a kernel of higher order  $\nu = Q + 1$  could be applied.

**Corollary 6.** Let the kernel k be spherically symmetric and  $Q \in \mathbb{N}$  odd. Under the conditions of Theorem 3, when searching for LOB in the space of isotropic candidates  $S = \{\sigma \mathcal{I}_d \mid \sigma > 0\}$ , and if all,  $p(x), v(x), bias_Q [x, \mathcal{I}_d] \neq 0$  do not vanish, then asymptotically it is

$$\Sigma_{Q}^{n}(x) = \sigma_{Asymp}^{Q,n}(x)\mathcal{I}_{d} + o_{p}\left[n^{-\frac{1}{2(Q+1)+d}}\right], \quad for$$
  
$$\sigma_{Asymp}^{Q,n}(x) = C_{Q}\left[\frac{v(x)}{p(x)n}\right]^{\frac{1}{2(Q+1)+d}} bias_{Q}\left[x,\mathcal{I}_{d}\right]^{-\frac{2}{2(Q+1)+d}}, \quad (15)$$

where  $C_Q = \left[ d \mathbf{R}_Q / \left( 2(Q+1) \right) \right]^{\frac{1}{2(Q+1)+d}}$  .

**Remark 7.** Corollary 6 and 8 will also hold for even order Q by replacing  $bias_Q[x, \mathcal{I}_d]$  with  $b_Q(x, \mathcal{I}_d)$  in the sense of Remark 4 and Q replaced by  $Q' = Q + (Q - 1 \mod 2)$  elsewhere.

The results of this section provide explicit forms of the asymptotic behavior of bias, variance and LOB that we can make use of in our work. From now on, we will restrict to the case of an odd LPS order Q, where we can apply a spherically symmetric kernel k. As discussed above, dealing with the case of even order Q is possible, yet unimportant in practice. In particular, for even order Q we can instead apply LPS of order (Q + 1), which is only marginally more complex and therefore poses no computational bottleneck.

## 2.2. Isotropic Optimal Sampling

We begin by simplifying our active learning objective (3) by rewriting  $\text{MSE}_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right)$  solely in terms of  $\mathbb{V}_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right)$ , which intuitively can be done because the LOB, as the optimal trade-off between bias and variance, will balance the error contribution of both components to the conditional MSE. We can support this intuition formally as follows (see also Zhang and Chan (2011)):

**Corollary 8.** Let the kernel k be spherically symmetric and  $Q \in \mathbb{N}$  odd. When applying  $\Sigma_Q^n(x)$  as the bandwidth for prediction in x, the conditional bias- and variance-related error components are asymptotically proportional over  $\mathcal{X}$ . That is, for all  $x \in \mathcal{X}$  it is

$$\mathbb{B}_Q\left(x, \Sigma_Q^n(x) | \boldsymbol{X}_n\right)^2 = \frac{d}{2(Q+1)} \operatorname{var}_Q\left[x, \Sigma_Q^n(x) \Big| \boldsymbol{X}_n\right] + o_p\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

Hence, the conditional MSE can asymptotically be expressed as

$$MSE_Q\left(x, \Sigma_Q^n(x) | \boldsymbol{X}_n\right) = \frac{2(Q+1)+d}{2(Q+1)} var_Q\left[x, \Sigma_Q^n(x) | \boldsymbol{X}_n\right] + o_p\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

Proof. Using Theorem 3 and Corollary 6, it is

$$\mathbb{B}_Q\left(x, \Sigma_Q^n(x) | \boldsymbol{X}_n\right) = \sigma_{\text{Asymp}}^{Q, n}(x)^{Q+1} \text{bias}_Q\left[x, \mathcal{I}_d\right] + o_p\left[n^{-\frac{Q+1}{2(Q+1)+d}}\right],$$

where it was  $\sigma_{\text{Asymp}}^{Q,n}(x) = C_Q \left[ v(x) / (p(x)n) \right]^{\frac{1}{2(Q+1)+d}} \text{bias}_Q \left[ x, \mathcal{I}_d \right]^{-\frac{2}{2(Q+1)+d}}$ . Furthermore, with (14),

$$\operatorname{var}_{Q}\left[x, \Sigma_{Q}^{n}(x) \middle| \mathbf{X}_{n}\right] = \mathbf{R}_{Q} \frac{v(x)}{p(x) n \sigma_{\operatorname{Asymp}}^{Q, n}(x)^{d}} + o_{p}\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

Therefore we can rewrite

$$\begin{split} &\mathbb{B}_{Q}\left(x, \Sigma_{Q}^{n}(x) | \boldsymbol{X}_{n}\right)^{2} + o_{p}\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right] = \sigma_{\text{Asymp}}^{Q,n}(x)^{2(Q+1)} \text{bias}_{Q}\left[x, \mathcal{I}_{d}\right]^{2} \\ &= C_{Q}^{2(Q+1)}\left[\frac{v(x)}{p(x)n}\right]^{\frac{2(Q+1)}{2(Q+1)+d}} \text{bias}_{Q}\left[x, \mathcal{I}_{d}\right]^{\frac{2d}{2(Q+1)+d}} \\ &= C_{Q}^{2(Q+1)+d}\left[\frac{v(x)}{p(x)n}\right] \sigma_{\text{Asymp}}^{Q,n}(x)^{-d} = \frac{d}{2(Q+1)} \text{var}_{Q}\left[x, \Sigma_{Q}^{n}(x) | \boldsymbol{X}_{n}\right]. \end{split}$$

Using Theorem 3, it is

$$MSE_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right) = \mathbb{B}_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right)^2 + \mathbb{V}_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right)$$
$$= \frac{2(Q+1) + d}{2(Q+1)} \operatorname{var}_Q\left[x, \Sigma_Q^n(x) | \mathbf{X}_n\right] + o_p\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

This result will become quite handy later on, as we can get rid of the cumbersome bias term, when estimating the conditional MSE at  $\Sigma_Q^n(x)$  in x.

Next, the asymptotic form in (15) reveals that LOB factorizes into a global scaling with respect to sample size n and local scaling components with respect to noise level v(x) and training density p(x). For Q odd, the last component  $\operatorname{bias}_{Q}[x, \mathcal{I}_{d}]$  solely contains information about the function f to be learnt near x. Intuitively, the optimal bandwidth will be locally smaller where the structure of f is locally more complex. Based on this observation, we define the following:

**Definition 9** (Isotropic complexity of LPS). For  $Q \in \mathbb{N}$  odd, let  $\Sigma_Q^n$  be the optimal bandwidth function as defined in (5). With the adjusted bandwidth function

$$\mathfrak{S}_{Q}^{n}(x) = C_{Q}^{-1} \left[ \frac{v(x)}{p(x)n} \right]^{-\frac{1}{2(Q+1)+d}} \Sigma_{Q}^{n}(x), \tag{16}$$

we define by

$$\mathfrak{C}_Q^n(x) = \left|\mathfrak{S}_Q^n(x)\right|^{-1} \tag{17}$$

the local function complexity (LFC) of f in x with respect to the LPS model of order Q.

Essentially, as the reciprocal of LOB,  $\mathfrak{C}_Q^n$  grows with increasing complexity of f, locally at x. But most importantly,  $\mathfrak{C}_Q^n$  is asymptotically independent of the global scaling with respect to training size n, as well as the local scaling with respect to the training density p and noise level v: Indeed, asymptotically we can write

$$\mathfrak{C}_Q^n(x) = \mathfrak{C}_Q^\infty(x)(1+o_p[1]), \text{ where } \mathfrak{C}_Q^\infty(x) = \operatorname{bias}_Q[x,\mathcal{I}_d]^{\frac{2d}{2(Q+1)+d}}.$$
 (18)

We observe that  $\mathfrak{C}_Q^n$  is asymptotically continuous, since  $\mathfrak{C}_Q^\infty$  is continuous via construction.

Combining the balancing property from Corollary 8 and the asymptotic results on LOB in Corollary 6 and the variance (14), we can express  $MSE_Q\left(x, \Sigma_Q^n(x) | \mathbf{X}_n\right)$  in terms of the training density p(x), the noise variance v(x), the training size n and the LFC  $\mathfrak{C}_Q^n(x)$ . With these preparations, we are now able to state our main result:

Let  $q \in \mathcal{C}^0(\mathcal{X}, \mathbb{R}_+)$  be a test density such that  $\int_{\mathcal{X}} q(x) dx = 1$ . Since  $\Sigma_Q^n$  is well-defined, recall from (6) that our active active learning objective is given by

$$\mathrm{MISE}_Q\left(q|\boldsymbol{X}_n\right) = \int_{\mathcal{X}} \mathrm{MSE}_Q\left(x, \Sigma_Q^n(x)|\boldsymbol{X}_n\right) q(x) dx.$$

Our goal is now to minimize  $\text{MISE}_Q(q|\mathbf{X}_n)$  with respect to the training set  $\mathbf{X}_n$ . As we will show in the following theorem, asymptotically, the optimal  $\mathbf{X}_n$  can be expressed as a random sample from the optimal density, which we denote by  $p_{\text{Opt}}^{Q,n}$ . That is,  $\mathbf{X}_n \sim p_{\text{Opt}}^{Q,n}$ .

**Theorem 10.** Let  $v, q \in C^0(\mathcal{X}, \mathbb{R}_+)$  for a compact input space  $\mathcal{X}$ , where q is a test density such that  $\int_{\mathcal{X}} q(x)dx = 1$ . Additionally, assume that v and q are bounded away from zero. That is,  $v, q \geq \epsilon$  for some  $\epsilon > 0$ . Let k be a RBF-kernel with bandwidth parameter space  $\mathcal{S} = \{\sigma \mathcal{I}_d \mid \sigma > 0\}$ . Let  $Q \in \mathbb{N}$  be odd and  $f \in C^{Q+1}(\mathcal{X})$  such that  $e_1^\top \mathbf{M}_Q^{-1} \mathbf{B}_Q \mathbf{D}_Q(x) \neq 0$ , almost everywhere. Then the optimal training density for LPS of order Q is asymptotically given by

$$p_{O_{pt}}^{Q,n}(x) \propto \left[\mathfrak{C}_Q^n(x)q(x)\right]^{\frac{2(Q+1)+d}{4(Q+1)+d}} v(x)^{\frac{2(Q+1)}{4(Q+1)+d}} (1+o(1)).$$
(19)

*Proof.* To begin with, recall from Corollary 6 that in the isotropic case, LOB is given by

$$\Sigma_Q^n(x) = \sigma_{\text{Asymp}}^{Q,n}(x)\mathcal{I}_d + o_p\left[n^{-\frac{1}{2(Q+1)+d}}\right],$$

where  $\sigma_{Asymp}^{Q,n}(x) = C_Q \left[ v(x) / (p(x)n) \right]^{\frac{1}{2(Q+1)+d}} \operatorname{bias}_Q \left[ x, \mathcal{I}_d \right]^{-\frac{2}{2(Q+1)+d}}$ . According to Corollary 8, it is

$$MSE_Q(x, \Sigma_Q^n(x) | \mathbf{X}_n) = \frac{2(Q+1) + d}{2(Q+1)} \operatorname{var}_Q[x, \Sigma_Q^n(x) | \mathbf{X}_n] + o_p[n^{-\frac{2(Q+1)}{2(Q+1) + d}}].$$

Noting that  $\left|\Sigma_Q^n(x)\right| = \sigma_{Asymp}^{Q,n}(x)^d$ , we know from (14) in Theorem 3 that

$$\operatorname{var}_{Q}\left[x, \Sigma_{Q}^{n}(x) \middle| \mathbf{X}_{n}\right] = \mathbf{R}_{Q} \frac{v(x)}{p(x)n} \left| \Sigma_{Q}^{n}(x) \right|^{-1}.$$

Using Definition 9 and (18), we can therefore write

$$\begin{split} \text{MSE}_{Q}\left(x, \Sigma_{Q}^{n}(x) | \boldsymbol{X}_{n}\right) \\ &= \frac{2(Q+1)+d}{2(Q+1)} \boldsymbol{R}_{Q} C_{Q}^{-d} \left[\frac{v(x)}{p(x)n}\right]^{\frac{2(Q+1)}{2(Q+1)+d}} \left|\mathfrak{S}_{Q}^{n}(x)\right|^{-1} + o_{p} \left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right] \\ &= \bar{C}_{Q} \left[\frac{v(x)}{p(x)n}\right]^{\frac{2(Q+1)}{2(Q+1)+d}} \mathfrak{C}_{Q}^{n}(x) + o_{p} \left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right] \\ &= \bar{C}_{Q} \left[\frac{v(x)}{p(x)n}\right]^{\frac{2(Q+1)}{2(Q+1)+d}} \mathfrak{C}_{Q}^{\infty}(x) + o_{p} \left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right], \end{split}$$

where we have set  $\bar{C}_Q = \frac{2(Q+1)+d}{2(Q+1)} R_Q C_Q^{-d}$ . Putting this into (6), we obtain

$$\operatorname{MISE}_{Q}\left(q|\boldsymbol{X}_{n}\right) = \int_{\mathcal{X}} \bar{C}_{Q}\left[\frac{v(x)}{p(x)n}\right]^{\frac{2(Q+1)}{2(Q+1)+d}} \mathfrak{C}_{Q}^{\infty}(x)q(x)dx + o_{p}\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

Since v,  $\mathfrak{C}_Q^{\infty}$  and q are continuous on the compact input space  $\mathcal{X}$ , the *Stone–Weierstrass theorem* guarantees a sequence  $g_Q^n \in \mathcal{C}^1(\mathcal{X})$  that satisfies

$$\sup_{x \in \mathcal{X}} \left| g_Q^n(x) - \left[ \frac{v(x)}{n} \right]^{\frac{2(Q+1)}{2(Q+1)+d}} \mathfrak{C}_Q^\infty(x) q(x) \right| < \frac{1}{n}.$$

Obviously,  $g_Q^n$  can be chosen independently of p. Hence we can write

$$\text{MISE}_{Q}\left(q|\boldsymbol{X}_{n}\right) = \int_{\mathcal{X}} \bar{C}_{Q} p(x)^{-\frac{2(Q+1)}{2(Q+1)+d}} g_{Q}^{n}(x) dx + o_{p} \left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right].$$

Define the Lagrangian for minimizing  $\text{MISE}_Q(q|\mathbf{X}_n)$  with respect to  $p \in \mathcal{C}^1(\mathcal{X}, \mathbb{R}_+)$  under the constraint  $\int_{\mathcal{X}} p(x) dx = 1$ , that is,

$$L(p,\lambda) = \int_{\mathcal{X}} \underbrace{\bar{C}_Q p(x)^{-\frac{2(Q+1)}{2(Q+1)+d}} g_Q^n(x) + \lambda p(x) dx - \lambda}_{F(x,p,\lambda)}.$$

We find the optimal training density to be  $p_{\text{Opt}}^{Q,n} := p^*$  for the stationary point  $(p^*, \lambda^*)$  of L that exhibits minimal objective. Note that since  $g_Q^n$ is continuously differentiable, so is F, such that we can apply calculus of variations to solve for extremes with respect to p:

$$0 = \frac{dF}{dp}(x) = -\frac{2(Q+1)\bar{C}_Q}{2(Q+1)+d}p(x)^{-\frac{4(Q+1)+d}{2(Q+1)+d}}g_Q^n(x) + \lambda$$
$$\Leftrightarrow p^*(x) = \left\{\frac{2(Q+1)\bar{C}_Q}{\lambda(2(Q+1)+d)}g_Q^n(x)\right\}^{\frac{2(Q+1)+d}{4(Q+1)+d}}$$

The concrete value of  $\lambda^*$  is not of interest. It is enough to guarantee  $\frac{dF}{d\lambda} = 0$  such that

$$p_{\text{Opt}}^{Q,n}(x) = \hat{C}_Q^{-1} g_Q^n(x)^{\frac{2(Q+1)+d}{4(Q+1)+d}} (1+o(1)),$$

where the normalization  $\hat{C}_Q = \int_{\mathcal{X}} g_Q^n(x)^{\frac{2(Q+1)+d}{4(Q+1)+d}} dx < \infty$  is bounded:

First of all let 
$$\hat{D}_Q = \int_{\mathcal{X}} v(x)^{\frac{2(Q+1)}{4(Q+1)+d}} \mathfrak{C}_Q^{\infty}(x)^{\frac{2(Q+1)+d}{4(Q+1)+d}} q(x)^{\frac{2(Q+1)+d}{4(Q+1)+d}} dx$$
. Note

that  $\hat{D}_Q < \infty$ , since v and  $\mathfrak{C}_Q^{\infty}$  are bounded over  $\mathcal{X}$ , and  $q \in L^{\frac{2(Q+1)+d}{4(Q+1)+d}}(\mathcal{X})$ since  $q \in L^1(\mathcal{X}) \subset L^{\frac{2(Q+1)+d}{4(Q+1)+d}}(\mathcal{X})$ . Thus,

$$\begin{split} \int_{\mathcal{X}} \left| g_Q^n(x) \right|^{\frac{2(Q+1)+d}{4(Q+1)+d}} dx &\leq \int_{\mathcal{X}} \left[ \left[ v(x)/n \right]^{\frac{2(Q+1)}{2(Q+1)+d}} \mathfrak{C}_Q^\infty(x) q(x) \right]^{\frac{2(Q+1)+d}{4(Q+1)+d}} dx \\ &+ \operatorname{Vol}(\mathcal{X}) n^{-\frac{2(Q+1)+d}{4(Q+1)+d}} = \hat{D}_Q n^{-\frac{2(Q+1)}{4(Q+1)+d}} (1+o(1)) < \infty \end{split}$$

Here, we defined by  $Vol(\mathcal{X}) = \int_{\mathcal{X}} dx$  the volume of  $\mathcal{X}$ , which is finite, since  $\mathcal{X}$  in compact. To summarize, asymptotically we can write

$$\begin{split} p_{\text{Opt}}^{Q,n}(x) &= \hat{C}_Q^{-1} g_Q^n(x)^{\frac{2(Q+1)+d}{4(Q+1)+d}} (1+o(1)) \\ &= \hat{D}_Q^{-1} v(x)^{\frac{2(Q+1)}{4(Q+1)+d}} \left[ \mathfrak{C}_Q^\infty(x) q(x) \right]^{\frac{2(Q+1)+d}{4(Q+1)+d}} (1+o(1)) \\ &= \hat{D}_Q^{-1} v(x)^{\frac{2(Q+1)}{4(Q+1)+d}} \left[ \mathfrak{C}_Q^n(x) q(x) \right]^{\frac{2(Q+1)+d}{4(Q+1)+d}} (1+o(1)). \end{split}$$

Note that, if  $\Sigma_Q^n$  is estimated based on  $\boldsymbol{X}_n \sim p_{\text{Opt}}^{Q,n}$ , then

$$p_{\text{Opt}}^{Q,n}(x) \propto \left\{ v(x)^{\frac{2(Q+1)}{2(Q+1)+d}} q(x) \left|\mathfrak{S}^{n}(x)\right|^{-1} \right\}^{\frac{2(Q+1)+d}{4(Q+1)+d}} \\ \propto \left\{ v(x)q(x)p_{\text{Opt}}^{n}(x)^{-\frac{d}{2(Q+1)+d}} |\Sigma_{Q}^{n}(x)|^{-1} \right\}^{\frac{2(Q+1)+d}{4(Q+1)+d}} \propto \left\{ v(x)q(x)|\Sigma_{Q}^{n}(x)|^{-1} \right\}^{\frac{1}{2}}.$$

The factorization (19) reveals the influence of the local function complexity, noise variance and test relevance of an input, which reflects human intuition: On the one hand, q(x) tells us about the relevance of an accurate prediction in x. Accordingly, we benefit from reinforcing the training set where q(x) is large. On the other hand, we require more samples where the noise variance v(x)or the local function complexity  $\mathfrak{C}_Q^n(x)$  is large. In addition, the factorization provides an exact quantitative result on how to account for each of these three factors in an optimal way.

**Remark 11.** When considering  $f \in C^{L+1}(\mathcal{X})$  with  $L \in \mathbb{N}$  odd, note that f is also a function of  $C^2(\mathcal{X}), \ldots, C^{L-1}(\mathcal{X})$  such that any LPS model of odd order  $1, 3, \ldots, L$  could be applied to calculate LFC (17) and the optimal training density (19). In practice, we will stick to low-order LPS models for computational tractability. However, due to the almost model-free nature of LPS, we consider these LFC and optimal training density of f that were obtained for the maximal applicable order as the 'true' LFC and optimal training density of f. That is, they represent properties that are intrinsic to f rather than the LPS model.

#### 2.3. The Active Learning Procedure

For now let us assume that we are given q,  $\mathcal{X}$  and reasonable estimates  $\widehat{\Sigma}_Q^n$ and  $\widehat{v}$  of LOB and the local noise level for any labeled training set  $\mathbf{X}_n, \mathbf{Y}_n$  of size n. Then we can formulate an online sampling procedure that approaches  $\mathbf{X}_n \sim p_{\text{Opt}}^{Q,n}$  as  $n \to \infty$ .

Let  $n_0$  be a small, but reasonable initial training size and  $p_0 \equiv \mathcal{U}(\mathcal{X})$ the initial training density according to which we sample the initial training inputs  $\mathbf{X}_{n_0}$  with labels  $Y_{n_0}$ . We then iterate over  $k \in \mathbb{N}_0$ , beginning with k = 0, to grow the training set as follows: Given the current training set  $\mathbf{X}_{n_k}, Y_{n_k}$  we estimate  $\hat{v}$  and  $\hat{\Sigma}_Q^{n_k}$ . Using (16), (17) and (19), it is

$$\begin{split} & \widehat{\mathfrak{C}}_Q^{n_k}(x) \propto \left[ \widehat{v}(x) \big/ p_k(x) \right]^{\frac{1}{2(Q+1)+d}} \left| \widehat{\Sigma}_Q^{n_k}(x) \right|^{-1}, \text{ and } \\ & \widehat{p}_{\text{Opt}}^{Q,n_k}(x) \propto \left[ \widehat{\mathfrak{C}}_Q^{n_k}(x) q(x) \right]^{\frac{2(Q+1)+d}{4(Q+1)+d}} \widehat{v}(x)^{\frac{2(Q+1)}{4(Q+1)+d}}. \end{split}$$

Setting  $n_{k+1} = 2n_k$ , we aim to draw  $X_{n_k+1}, \ldots, X_{n_{k+1}} \sim \tilde{p}_{k+1}$  such that the new training set  $X_{n_{k+1}} \sim p_{k+1}$  is as close to the proposed optimal training density estimate  $\hat{p}_{\text{Opt}}^{Q,n_k}$  in distribution as possible:

Writing  $p_{k+1} := \gamma_2 p_k + (1 - \gamma_2) \hat{p}_{\text{Opt}}^{Q,n_k}$ , we therefore aim to minimize  $\gamma_2 \in [0, 1]$ . Note that we could simply set  $\tilde{p}_{k+1} \equiv \hat{p}_{\text{Opt}}^{Q,n_k}$ , that is, sampling the new batch according to the current proposed optimal training density estimate. In this case we get  $\gamma_2 = 0.5$ . However, a stronger similarity of  $p_{k+1}$  to  $\hat{p}_{\text{Opt}}^{Q,n_k}$  is always possible: Define  $p_{k+1} := \gamma_2 p_k + (1 - \gamma_2) \hat{p}_{\text{Opt}}^{Q,n_k}$ , where

$$\gamma_1 = \max_{x \in \mathcal{X}} \frac{p_k(x)}{\hat{p}_{\text{Opt}}^{Q, n_k}(x)} \in [1, \infty) \quad \text{and} \qquad \gamma_2 = \max\left\{0, \frac{0.5 - \gamma_1^{-1}}{1 - \gamma_1^{-1}}\right\} \in [0, 0.5).$$

Then we obtain  $X_{n_{k+1}} \sim p_{k+1}$  by drawing  $X_{n_k+1}, \ldots, X_{n_{k+1}} \sim \tilde{p}_{k+1}$  for  $\tilde{p}_{k+1} = 2p_{k+1} - p_k$ . Note that  $\tilde{p}_{k+1}$  is a valid probability density, because

$$\int_{\mathcal{X}} \widetilde{p}_{k+1}(x) dx = 2 \int_{\mathcal{X}} p_{k+1}(x) dx - \int_{\mathcal{X}} p_k(x) dx = 2 - 1 = 1,$$

and  $\widetilde{p}_{k+1} \geq 0$ : Indeed, for any  $x \in \mathcal{X}$ , it is

$$p_{k+1}(x)/p_k(x) = \gamma_2 + (1-\gamma_2)\hat{p}_{\text{Opt}}^{Q,n_k}(x)/p_k(x) \ge \gamma_2 + (1-\gamma_2)\gamma_1^{-1}$$
$$= \gamma_2(1-\gamma_1^{-1}) + \gamma_1^{-1} \ge \frac{0.5-\gamma_1^{-1}}{1-\gamma_1^{-1}}(1-\gamma_1^{-1}) + \gamma_1^{-1} = 0.5.$$

Therefore  $2p_{k+1}(x) \ge p_k(x)$  such that  $\tilde{p}_{k+1}(x) = 2p_{k+1}(x) - p_k(x) \ge 0$ .

#### 3. Practical Considerations

While the theoretical result above is an insightful contribution on its own, one may ask about its relevance in practice, since on first glance we require a lot of information about the true data distribution. This information is especially scarce in the early stages of active learning, where we only have access to a small set of labeled instances.

First of all, we would like to emphasize that, while we rely on the explicit formulation of bias in our theoretical analysis, our results will apply to any consistent estimate of  $\Sigma_O^n(x)$ .

Recalling (15), it is possible to construct LOB via the bias which involves the estimation of  $D_f^{Q+1}(x)$ . Yet, this approach is of very limited relevance: Even though we search over the restricted space of isotropic bandwidths  $S = \{\sigma \mathcal{I}_d, \sigma > 0\}$ , which has only one degree of freedom, the number of components of the derivative to fit grows as  $O(d^{Q+1})$ . This quickly becomes computationally intractable as d increases: For example, when considering its estimation via LPS (Zhang and Chan, 2011), it involves solving a linear system of the size of the number of the derivative components, which is  $O(d^{3(Q+1)})$ . Moreover, even estimates of lower order derivatives like the Hessian require a large amount of training data. In our experiments, we use Lepski's method (Lepski, 1991; Lepski and Spokoiny, 1997), which is a direct estimate to LOB that avoids these difficulties. We detail this approach in Sec. 3.2.

With respect to the other two quantities, namely local noise variance v(x)and test density q(x), we would like to emphasize that we do not necessarily require full estimates for them: In the case where homoscedasticity is (or can be) assumed, we only have to estimate a constant  $v(x) \equiv v$ . Whether we need a local estimate v(x) or the global estimate v, we discuss a simple approximation in Sec. 3.1, which then serves as an input to Lepski's method. Finally regarding q(x), there are two major scenarios: We might know  $\mathcal{X}$  and the test density q(x) is externally specified – therefore requires no estimation. Here, the canonical candidate is the uniform distribution  $q \sim \mathcal{U}(\mathcal{X})$ , where we aim to optimize the prediction performance uniformly well over the input space.

In the other scenario, we observe inputs  $x \sim p_{\chi}$  from an unknown data generating process. Here, the natural candidate for the test density  $q \equiv p_{\chi}$ , and we require an estimate  $\hat{p}_{\chi}$ . In this scenario – also known as *pool-based* active learning – it is a common assumption that unlabeled input instances are cheaply obtainable in contrast to labeled samples. Therefore we can estimate  $\hat{p}_{\chi}$  in advance, prior to the actual active learning procedure. We refer to the broad literature on density estimation Silverman (1986); Wand and Jones (1994) in this case.

## 3.1. Estimation of the local Noise Variance

Regarding the estimation of the local noise variance v(x), we first consider the homoscedastic scenario for d=1, where  $v(x) \equiv v$ . Here, a robust estimate to v based on the *median absolute deviation* (MAD) is known (see, for example, Katkovnik et al. (2006)):

$$\sqrt{\hat{\mathbf{v}}} = (\sqrt{2} \cdot 0.6745)^{-1} \operatorname{median}(\{|y_{\pi(i)} - y_{\pi(i+1)}| \mid 0 < i < n\}), \qquad (20)$$

where  $\pi$  is an ordering index permutation such that  $x_{\pi(i)} < x_{\pi(i+1)}$  for 0 < i < n. The MAD estimate (20) relies on the fact that  $y_{\pi(i)} - y_{\pi(i+1)} \rightarrow \varepsilon_{\pi(i)} - \varepsilon_{\pi(i+1)}$  as  $n \rightarrow \infty$ . The idea may fail at small sample sizes where

 $|f(x_{\pi(i)}) - f(x_{\pi(i+1)})| \gg \epsilon ||f||$  for some considerable constant  $\epsilon > 0$ . This is critical as it influences the subsequent sampling process in a negative way. We tackle this issue by replacing  $y_i$  above with the residuals  $r_i = y_i - \hat{f}^{\sigma}(x_i)$  for a global predictor  $\hat{f}^{\sigma}(x) = m_Q^{\sigma \mathcal{I}_d}(x)$  according to the LPS model (9), for which we cross-validate the constant bandwidth  $\sigma$  over the current training set.

As a generalization of (20) to both, higher dimensions d > 1 and heteroscedasticity, let  $\mathcal{J}_m^i \subseteq \mathbf{X}_n$  be the set of indices of the m-nearest neighbors of  $x_i$  in  $\mathbf{X}_n$ , and for an arbitrary  $x \in \mathcal{X}$  let  $\mathcal{I}_l(x) \subseteq \mathbf{X}_n$  be the indices of the l-nearest neighbors of x in  $\mathbf{X}_n$ . Then we estimate

$$\sqrt{\widehat{v}(x)} = (\sqrt{2} \cdot 0.6745)^{-1} \operatorname{median} \bigcup_{i \in \mathcal{I}_l(x)} \bigcup_{j \in \mathcal{J}_m^i} |r_i - r_j|.$$
(21)

While *m* is a free parameter, we set m = 2d in the following. For asymptotic consistency of the estimate, the number of neighbors  $l := l_n$  should increase with n, but  $l_n \in o(n)$  such that the expected diameter of the neighborhoods  $\{x_j \mid j \in \mathcal{J}_m^i\}$  decreases for all *i*. For an optimal trade-off, note that according to Foi (2007) (page 161), it is  $\mathbb{E}(\sqrt{\hat{v}(x)}) = \sqrt{v(x)}$  and  $\mathbb{V}(\sqrt{\hat{v}(x)}) \approx 1.35v(x)/((l-1)+1.5)$ . Furthermore, according to Evans et al. (2002),  $\mathbb{E}|x_i - x_j| \leq (m/n)^{\frac{1}{d}}$  for  $j \in \mathcal{J}_m^i$ , and analogously  $\mathbb{E}|x_i - x_j| \leq (l/n)^{\frac{1}{d}}$  for  $i \in \mathcal{I}_l(x)$ . Therefore

$$\mathbb{E}\left[(\sqrt{\widehat{v}(x)} - \sqrt{v(x)})^2 | \mathbf{X}_n\right] \le \underbrace{v(x) \frac{1.35}{l+0.5}}_{O(l^{-1})} + \underbrace{\|D_f\|_{\infty}^2 \left(\frac{m}{n}\right)^{\frac{2}{d}} + \|D_v\|_{\infty}^2 \left(\frac{l}{n}\right)^{\frac{2}{d}}}_{O(\left(\frac{l}{n}\right)^{\frac{2}{d}})}.$$

For fastest convergence, we need to balance both error components, giving the optimal relation  $l_n = \lceil C_v n^{\frac{2}{2+d}} \rceil$  in the heteroscedastic case for some reasonably chosen constant  $C_v > 0$ . When we have expert knowledge about homoscedasticity, we apply (21) with  $l_n = n$ , forcing it to become a global estimate again.

#### 3.2. Estimation of the locally Optimal Bandwidths

Lepski et al. (Lepski, 1991; Lepski and Spokoiny, 1997) considered optimal pointwise adaptation in the broader context of nonparametric estimation. We will follow the work of Zhang and Chan (2011), who implemented Lepski's method for LPS.

Consider a set of logarithmically spaced bandwidth candidates, that is,  $\Sigma_0, \ldots, \Sigma_L$  with  $\Sigma_j = \sigma_j \mathcal{I}_d$  and  $\sigma_j = \underline{\sigma} \cdot s^j$  for a step size s > 1 and a lower bound  $\underline{\sigma}$ . For an  $x \in \mathcal{X}$  we choose  $\widehat{\Sigma}_Q^n(x)$  according to the *intersection of* confidence interval (ICI) rule: Let

$$\mathcal{C}_{Q}^{j}(x) = \left\{ c \in \mathbb{R} \ \left| \ |c - m_{Q}^{\Sigma_{j}}(x)| \le \kappa (1 + 2/(s^{\frac{2(Q+1)+d}{2}} - 1)) \sqrt{\mathbb{V}_{Q}(x, \Sigma_{j} | \mathbf{X}_{n})} \right. \right\}$$

be the confidence interval constructed such that  $\mathbb{E} m_Q^{\Sigma_j}(x) \in \mathcal{C}_Q^j(x)$  with high probability, where we can calculate the prediction variance  $\mathbb{V}_Q(x, \Sigma_j | \mathbf{X}_n)$ according to (12). For example, for  $\kappa = 1.96$  and  $\kappa = 2.58$  it is  $\mathbb{P}(m_Q^{\Sigma_j}(x) \in \mathcal{C}_Q^j(x)) = 0.95$  and 0.99, respectively. Furthermore let

$$j^*(x) = \max\left\{0 \le j \le L \mid \bigcap_{i \le j} \mathcal{C}_Q^i(x) \ne \emptyset\right\},\$$

meaning that for  $j > j^*(x)$  the confidence intervals do not intersect anymore. We then set

$$\widehat{\Sigma}^n_Q(x) = \Sigma_{j^*(x)}.$$
(22)

Commonly, the bandwidth candidate parameters are set to  $s = 2, \underline{\sigma} > 0$  fixed to a small value, and L such that  $\sigma_L \leq n/\log(n)$ . We will however choose  $\underline{\sigma}_n$  and  $s_n$  adaptively: For some reasonable constant  $C_{\sigma} > 0$  we set  $\underline{\sigma}_n = C_{\sigma}n^{-\frac{2}{2(Q+1)+d}}$ , which decays twice as fast as the usual bandwidth decay rate, enabling us to reproduce fine structure that may first reveal at larger training sizes. Furthermore, noting that the confidence interval range is proportional to  $n^{-\frac{Q+1}{2(Q+1)+d}} / \left[s_n^{\frac{2(Q+1)+d}{2}} - 1\right]$ , we set  $s_n = \left[1 + C_s n^{-\frac{Q+1}{2(Q+1)+d}}\right]^{\frac{2}{2(Q+1)+d}}$  such that  $s_n$  decays, but slow enough to not blow up the confidence intervals as n increases. Here,  $C_s > 0$  is a reasonable constant. For example, with  $C_s = n_0^{\frac{Q+1}{2(Q+1)+d}} (2^{\frac{2(Q+1)+d}{2}} - 1)$  we obtain  $s_{n_0} = 2$ .

#### 3.3. Stabilization of local Estimates

At small training size n, the effective number of samples that are involved in the estimation of  $\hat{\Sigma}_Q^n$  and  $\hat{v}$  can be marginal which may result in quite unstable estimates. In an online procedure, where we add new samples according to our proposed optimal training density that relies on these estimates, such instability is critical: Given a faulty estimate of small noise or complexity (a large bandwidth) in x, we might end up in a singular case, where we add no further sample in the vicinity of x for a long time.

In order to prevent this, we suggest to replace the pointwise estimates of the noise level and LOB most conservatively as follows: Let  $B_{\delta_n}(x) =$   $\{x' \in \mathcal{X} \mid ||x - x'|| \leq \delta_n\}$  be the ball around x of radius  $\delta_n$ . We replace the estimate  $\hat{v}(x)$  from (21) by

$$\widetilde{v}(x) = \max\left\{\widehat{v}(x') \mid x' \in B_{\delta_n}(x)\right\}.$$
(23)

Similarly, we replace  $\widehat{\Sigma}_Q^n(x)$  in (22) by

$$\widetilde{\Sigma}_Q^n(x) = \Sigma_{\tilde{j}^*(x)}, \quad \text{where}$$

$$\tilde{j}^*(x) = \min\left\{ 0 \le j \le L \mid \exists x' \in B_{\delta_n}(x) : \widehat{\Sigma}_Q^n(x) = \Sigma_j \right\}.$$
(24)

This is conservative in the sense that we tend to overestimate the local noise level and local function complexity, which results in more sample mass in the subsequent sampling step.

For asymptotic optimality it must hold  $\delta_n \to 0$  as  $n \to \infty$ . On the other hand,  $\delta_n$  should decay slow enough such that the expected number of training samples in  $B_{\delta_n}(x)$  increases. Thus, it must hold  $\delta_n = \omega_p \left[n^{-\frac{1}{d}}\right]$ , and we choose  $\delta_n = C_{\delta} n^{-\frac{1}{d(d+1)}}$  for some reasonable constant  $C_{\delta} > 0$ .

#### 3.4. Boundary Correction of the Optimal Training Density

Even though Theorem 10 holds asymptotically almost everywhere, for finite training size n there will be an undesired behavior at the support boundary: While for odd-order Q the MSE convergence law at the support boundary is consistent with the law in the interior of the support, the conditional bias and variance behave differently to equations (13) and (14) in a non-trivial way. Asymptotically, this can be ignored as the support boundary makes up a set of measure zero. Yet, for finite n, the support boundary has substantial measure and we suggest to perform a correction of the proposed optimal training density estimate:

Let  $\mathfrak{s} > 0$  be some reasonable factor of the standard deviation to the kernel k such that

$$\int_{B_{\mathfrak{s}}(0)} k(u) du = 1 - \varepsilon$$

for some small  $\varepsilon > 0$ . For example, for the Gaussian kernel we may apply a value of  $1 \leq \mathfrak{s} \leq 3$ . At training size n, we define the effective support interior  $\mathcal{X}_n^{\circ}$  of  $\mathcal{X}$  as

$$\mathcal{X}_{n}^{\circ} = \left\{ x \in \mathcal{X} \mid \left\{ x' \in \mathbb{R}^{d} \mid \| [\Sigma_{Q}^{n}(x)]^{-1}(x - x') \| \leq \mathfrak{s} \right\} \subset \mathcal{X} \right\}.$$
(25)

Note that for any  $\mathfrak{s}>0$  ,  $\mathcal{X}_n^\circ\to\mathcal{X}^\circ$  as  $n\to\infty.$  As a correction, we suggest to set

$$\widetilde{p}_{\text{Opt}}^{Q,n}(x) = \begin{cases} \widehat{p}_{\text{Opt}}^{Q,n}(x) & , x \in \mathcal{X}_{n}^{\circ}, \\ \widehat{p}_{\text{Opt}}^{Q,n}(x_{n}^{\circ}) & , \text{else, where } x_{n}^{\circ} = \operatorname{arg\,min}_{x' \in \mathcal{X}_{n}^{\circ}} \|x - x'\|. \end{cases}$$
(26)

#### 3.5. Algorithmic Summary

Let us recapitulate that we require reasonable constants  $C_v$  for the localization of the noise estimate,  $C_{\sigma}$  and  $C_s$  for the lower bandwidth candidate bound and the step size of the bandwidth candidates, and the confidence interval size factor  $\kappa$  in Lepski's method. Furthermore, we require the constants  $C_{\delta}$  for stabilization of the local property estimates, and the standard deviations factor  $\mathfrak{s}$  of the kernel to identify regions of the input space that will suffer from boundary effects at finite training sizes. Given these constants, we have summarized a full active learning step of our proposed framework in Algorithm 1.

## Algorithm 1 Construction of $(X_{n_{k+1}}, Y_{n_{k+1}})$ from $(X_{n_k}, Y_{n_k})$

#### Input

- 1: Current training inputs  $X_{n_k}$  with labels  $Y_{n_k}$  and training density  $X_{n_k} \sim p_k$
- 2: The test density q
- 3: The order Q of the underlying LPS model
- 4: Constants  $C_v$  for the localization of the noise estimate,  $C_s$  and  $C_{\sigma}$  for Lepski's bandwidth candidate step size factor  $s_n$  and the smallest candidate  $\underline{\sigma}_n$  and  $C_{\delta}$  for choosing the local estimates stabilizer  $\delta_n$
- 5: The confidence interval size factor  $\kappa$  of Lepski's method and the standard deviations factor  $\mathfrak{s}$  of the kernel for boundary correction of the optimal training density estimate

6: A Boolean homoscedastic, if homoscedastic noise can be assumed Output 7: New training inputs  $\pmb{X}_{n_{k+1}}$  with labels  $Y_{n_{k+1}}$  and training density  $\pmb{X}_{n_{k+1}} \sim p_{k+1}$ Procedure 8: if homoscedastic then ▷ Set training size dependent parameters  $l_{n_k} = n_k \text{ else } l_{n_k} = C_v n_k^{\frac{2}{2+d}}$ 9:  $s_{n_k} = \left[1 + C_s n_k^{-\frac{Q+1}{2(Q+1)+d}}\right]^{\frac{2}{2(Q+1)+d}}, \underline{\sigma}_{n_k} = C_\sigma n_k^{-\frac{2}{2(Q+1)+d}}, \delta_{n_k} = C_\delta n_k^{-\frac{1}{d(d+1)}}$ 10: Estimate  $\hat{v}$  according to (21), using  $X_{n_k}, Y_{n_k}$  and neighborhood size  $l_{n_k} \triangleright$  see Sec. 3.1 11: Obtain the stabilized noise estimate  $\tilde{v}$  according to (23), using  $\delta_{n_k}$  $\triangleright$  see Sec. 3.3 12: Estimate LOB  $\widehat{\Sigma}_Q^{n_k}$  via Lepski's method (22),  $\triangleright$  see Sec. 3.2 using  $\boldsymbol{X}_{n_k}, Y_{n_k}, \widetilde{v}, \kappa, s_{n_k}$  and  $\underline{\sigma}_{n_k}$ 13: Obtain the stabilized LOB estimate  $\tilde{\Sigma}_Q^{n_k}$  according to (24), using  $\delta_{n_k} \quad \triangleright$  see Sec. 3.3 14: Estimate  $\hat{p}_{\text{Opt}}^{Q,n_k}$  according to (16), (17) and (19)  $\triangleright$  see Sec. 2.3 15: Perform boundary correction (26) to obtain  $\widetilde{p}_{\mathrm{Opt}}^{Q,n_k}$  $\triangleright$  see Sec. 3.4 16: Set  $\gamma_1 = \max_{x \in \mathcal{X}} p_k(x) / \tilde{p}_{\text{Opt}}^{Q,n_k}(x)$  and  $\gamma_2 = \max\left\{0, (0.5 - \gamma_1^{-1}) / (1 - \gamma_1^{-1})\right\}$ 17: Set  $p_{k+1} = \gamma_2 p_k + (1 - \gamma_2) \tilde{p}_{\text{Opt}}^{Q,n_k}$  $\triangleright$  see Sec. 2.3 18: Sample  $X_{n_k+1}, \ldots, X_{n_{k+1}} \sim \widetilde{p}_{k+1}$ , where  $\widetilde{p}_{k+1} = 2p_{k+1} - p_k$ , to obtain  $X_{n_{k+1}} \sim p_{k+1}$ 19: Query the labels  $y_{n_k+1}, \ldots, y_{n_{k+1}}$  of  $X_{n_k+1}, \ldots, X_{n_{k+1}}$  to obtain  $Y_{n_{k+1}}$ 

### 4. Discussion and Related Work

We will now elaborate the active learning properties mentioned in the introduction in more detail and show that our proposed methodology encompasses all of them. Additionally, we will discuss related work in the light of these properties.

#### 4.1. The Active Learning Properties

Let us recall from Sec. 1 that – besides the fundamental categories of (un)supervised and model-free/based sampling schemes – the most relevant properties of sampling schemes in the scope of this work are *optimality*,

robustness and model-agnosticity. We have also motivated why it is preferable to have a sampling scheme that possesses these three properties at the same time. We will now discuss these three properties and their relation in more detail. In particular, we will conclude that a sampling scheme has to be necessarily supervised and nonparametric in order to fulfill them simultaneously.

First of all note that the difference between a *robust* and a *model-agnostic* sampling scheme is subtle: Especially in the parametric regime, both properties never hold, making them coincide trivially. In contrast, in the nonparametric regime, let us consider uncertainty sampling for standard Gaussian process regression (GPR) (Seo et al., 2000), where new samples are drawn so as to minimize the integrated predictive variance. By standard GPR we mean a Gaussian process that is based on a global bandwidth parameter that allows for no local adaption. Here, the bias is assumed to be negligible, compared to the variance, and thus can be completely ignored. For those regression problems where the assumption of a negligible bias is justified, GPR uncertainty sampling is an *optimal* sampling scheme for GPR and superior to *random* test sampling across model classes, making it a model-agnostic sampling scheme. Ignoring the bias is however incorrect for regression problems of inhomogeneous complexity structure, where the bias varies over the input space. Since standard GPR uncertainty sampling does not account for this inhomogeneity, it is not an appropriate sampling scheme for GPR or other model classes. As in practice inhomogeneously complex regression problems occur frequently (Donoho and Johnstone, 1994; Benesty and Huang, 2013) the assumption of a negligible bias is not a mild one. In this light, standard GPR uncertainty is not *robust*.

As we have already discussed in the introduction, it is somewhat contradictory for a sampling scheme to be *optimal* on the one hand, and *robust* and *model-agnostic* on the other hand. In fact, in the unsupervised regime *robustness* and *optimality* are mutually exclusive:

**Lemma 12.** A sampling scheme cannot be optimal, robust and unsupervised, simultaneously.

*Proof.* Assume by contradiction that there exists an *optimal*, *robust* and unsupervised sampling scheme. Since it is *optimal*, it must be model-based. This model  $\hat{f}$  must be nonparametric, due to *robustness*, and it must treat bias and variance. Now assume some arbitrary input space  $\mathcal{X}$ . Since the sampling scheme is unsupervised,  $(\hat{f}, \mathcal{X})$  already uniquely determine the associated optimal training distribution  $\mathbf{X}_n \sim p_n^{\text{train}}$ . Since  $\hat{f}$  is nonparametric, itself as well as  $p_n^{\text{train}}$  are local. That is, for subsets  $\mathcal{A} \subset \mathcal{X}$  the optimal training density

of the restriction  $\hat{f}|_{\mathcal{A}}$  is given by  $p_n^{\text{train}}|_{\mathcal{A}}$ . Now, robustness and optimality imply that  $p_n^{\text{train}}$  is optimal for a substantial space of label distribution p(y|x), whereas it is not optimal for a negligible space of labelings. Optimal means that  $\mathbf{X}_n$  minimizes, for example, the MISE for such a labeling p(y|x).

Without loss of generality we assume that  $p_n^{\text{train}} \not\sim \mathcal{U}(\mathcal{X})$ , because  $\mathcal{U}(\mathcal{X})$ is an optimal solution for a set of labelings of measure zero in the space of heteroscedastic and inhomogeneously complex problems. Then there necessarily exists a reflection  $R_{\bar{x}}$  in  $\bar{x} \in \mathcal{X}^\circ$  with  $B_{\varepsilon}(\bar{x}) \subset \mathcal{X}$  for some  $\varepsilon > 0$ such that  $p_n^{\text{train}} \circ R_{\bar{x}}|_{B_{\varepsilon}(\bar{x})} \not\equiv p_n^{\text{train}}|_{B_{\varepsilon}(\bar{x})}$ . We now construct the new labeling  $p^*(y|x) = \begin{cases} p(y|R_{\bar{x}}(x)), & x \in B_{\varepsilon}(\bar{x}) \\ \widetilde{p}(y|x), & \text{else} \end{cases}$  over  $\mathcal{X}$ , where we can choose  $\widetilde{p}(y|x)$  as a continuation of  $p(y|R_{\bar{x}}(x))$  outside  $B_{\varepsilon}(\bar{x})$  that preserves the regularity of p(y|x). By construction,  $p_n^{\text{train}}$  is not the optimal training distribution for  $p^*(y|x)$ , because of the locality of  $\widehat{f}$  and  $p_n^{\text{train}}$ . Now that the choice of p(y|x)

was arbitrary, we have a substantial set of labelings  $p^*(y|x)$  on  $\mathcal{X}$  for which

 $p_n^{\text{train}}$  is not *optimal*, in contradiction to the assumption.

For example, there exist model-based, *optimal* sampling schemes that are also unsupervised – that is, they do not depend on labels even if some labeled samples are available, like in optimum experimental design (Kiefer, 1959; MacKay, 1992; He, 2010) and in uncertainty sampling for GPR (Seo et al., 2000). In the light of Lemma 12, these sampling schemes are necessarily not *robust*, which means that they must impose strong assumptions on the regularity of the labels. In fact, particularly these strong assumptions are necessary to make such sampling schemes unsupervised.

Second, sampling schemes based on parametric models are quite specific to the model and are therefore never *model-agnostic*. As a compromise between model-free and parametric approaches, nonparemetric models impose rather mild conditions on the labels. Thus, a sampling scheme based on a nonparametric model is more promising, though not guaranteed, to be *model-agnostic*. Finally, advanced model-free sampling schemes (Teytaud et al., 2007) are inherently *model-agnostic* and *robust*, because they were not derived via a model that might assume any regularity of the labels. However also by definition, they are necessarily not *optimal*, because of the absence of such a model.

To summarize, we sketch the relation between *optimal*, *robust* and *model-agnostic* sampling schemes, as well as (un)supervised and (non)parametric sampling schemes in Fig. 4.1, where we also exemplarily classify the discussed active learning approaches from related work. The goal of our work was



Figure 1: Relation between the main properties of active learning approaches we focus on in this work. The filled, purple area contains the candidates for our purpose.

to propose a sampling scheme that combines the amenities of both sides, model-free and *optimal* approaches. Namely, it should lead to a consistent performance increase across several model classes, while being truly adapted to the regression task at the same time. Therefore it has to be simultaneously *optimal*, *robust* and *model-agnostic*.

With the above arguments we can narrow down the set of candidate sampling schemes as claimed: Namely, such a sampling scheme must be model-based, since model-free sampling schemes are never *optimal*. Next, since parametric sampling schemes are never *model-agnostic*, the candidate must be necessarily nonparametric. Finally, in order to additionally match *robustness*, we need a supervised sampling scheme since *robustness* and *optimality* are incompatible in the unsupervised regime.

In addition, our sampling scheme is *stationary* and *interpretable*:

Further properties of sampling schemes: We call a sampling scheme

- **stationary**, if the training inputs can be formulated as an independently and identically distributed random sample of a fixed distribution.
- **interpretable**, if the decision making on which labels to query can be visualized to and understood by a domain expert.

A stationary sampling scheme shares the benefits of unsupervised sampling schemes, when the desired terminal training size is large, or when the annotator of the label queries, such as a human expert, is not always available (Settles, 2010). For a *stationary* sampling scheme, the data acquisition can be proceeded independently from data annotation – even if supervised. In contrast, for example, information-based sampling schemes (MacKay, 1992) require re-estimation of the information measure after the acquisition of each new sample.

The advantage of an *interpretable* sampling scheme is that we can give an explanation for what reason a proposed query seems informative, which a human expert is able to comprehend. In this case, a domain expert is able to monitor the healthiness of the sampling process, as opposed to a black box sampling process where a potential faulty behavior will reveal in hindsight (Lapuschkin et al., 2019; Samek et al., 2021). Therefore, such transparency makes active learning more appealing in real-world environments, where data acquisition and annotation is expensive, as we can reduce the risk of wasting costs.

## 4.2. Properties of the Proposed Sampling Method

Our proposed sampling scheme fulfills all five introduced properties:

(**optimal**) Theorem 10 guarantees that, asymptotically, our proposed sampling scheme is the solution to (4), the minimal MISE of the LPS model, which proves optimality.

(**robust**) In order to asymptotically minimize MISE, we rely on the expressions of the leading-order bias- and variance-terms as given in Theorem 3. Therefore, we assume certain smoothness of the noise level, the test density and the function to learn, as well as non-vanishing leading terms, almost everywhere. All these assumptions are mild (as opposed to assuming homoscedasticity or a negligible bias), which makes our sampling scheme *robust*.

(model-agnostic) As already mentioned, our sampling scheme is likely to provide the *model-agnosticity*, since the LPS model as the base of our objective is almost model-free. We will show in the experiments in Sec. 5 that this property indeed holds.

(stationary) Since  $p_{\text{Opt}}^{Q,n}$  converges in probability to an asymptotic density, our sampling scheme  $X_n^* \sim p_{\text{Opt}}^{Q,n}$  is asymptotically stationary. Hence, it features the stationarity property.

(interpretable) Instead of having to rely on a black box information score, the closed-form solution of  $p_{\text{Opt}}^{Q,n}$  reveals influence of LFC, noise variance and

test density on the optimal sample. These three scalar-valued properties can intuitively be understood by a human expert, which makes our sampling scheme *interpretable*.

### 4.3. Related Work

Recall that our proposed active learning scheme is *optimal*, *robust* and *model-agnostic*, among other properties. It is therefore especially well designed for the mid- to long-term construction of a meaningful training set in regression tasks where there is scarce domain knowledge, such that we only know few about the regularity of the problem and/or have not determined the final regression model to solve the problem optimally. However, as we have deduced in Sec. 4.1, an approach with the specification of our proposed sampling scheme is necessarily supervised. And like any supervised sampling scheme, we thus require a small, but sufficient amount of training labels for the initial estimation of the sampling criterion.

This initialization could be done by random test sampling, but also by any reasonable unsupervised sampling scheme – as suggested by Liu et al. (2021). Especially, for the reasons of a consistent performance increase and model flexibility, unsupervised, input space geometric sampling schemes enjoy great popularity (Teytaud et al., 2007; Yu and Kim, 2010; Wu, 2019; Liu et al., 2021) in practice. As they are model-free, they are inherently model-agnostic and *robust* by definition. However also by definition, they are necessarily not optimal, and thus become inferior to optimal sampling schemes in the long run: For example Teytaud et al. (2007) aim to make the training set as diverse as possible. While such approaches show advantages in the early stages of the training set construction, they become inferior to *optimal* sampling schemes as soon as the input space is well represented. In summary, unsupervised, input space geometric sampling schemes and sampling schemes with the same specification as our proposed framework play a complementary role: While both categories are *robust* and *model-aquostic*, the prior one works from scratch, whereas the latter one is *optimal*.

Let us also take a look at unsupervised, model-based sampling schemes that could be used, among other things, for the initialization of a supervised sampling scheme. Model-based, unsupervised approaches eliminate the dependence on the labels by imposing strong model assumptions. For example, in linear parametric regression a correct model specification is assumed such that bias can be considered negligible: Here, the minimization of the expected generalization loss can be translated to maximizing information gain. Some approaches encode information via the variance of the model parameters at the current training state (see, for example, Sugiyama and Nakajima (2009)). Also the theory of optimum experimental design (see, for example, Kiefer (1959)) follows this approach, using the *Fisher information* as a measure to minimize the variance. These methods have since been extended beyond simple linear methods to kernel methods and modified to take into account regularization (see He (2010)). MacKay (1992) follow this idea in a Bayesian setting. In the nonparametric regime such as Gaussian process regression, Seo et al. (2000) assume strong correlation between the shape of the applied kernel and the predictive variance.

A parametric, unsupervised approach is not *model-agnostic*, making it no good candidate for the initialization of a supervised approach. Additionally, both, parametric and nonparametric, unsupervised approaches are not *robust* in our definition. Therefore also a nonparametric, unsupervised should be applied with caution when there is almost no domain knowledge that may justify the model assumptions. On the other hand, when the model assumptions are justified the respective models can also serve reasonably as the final prediction model. Especially a parametric approach has a MISE that decays at the rate  $O(n^{-1})$ , which is superior to the convergence of any nonparametric model.

Unsupervised sampling schemes often do not require intensive recalculations of the sampling criterion after each query. Additionally, as they do not rely on the labels to query, they will not suffer from a potential bottleneck at the label annotation, which could, for example, be a human that is not always available. Therefore they share the essential benefits of a stationarity sampling scheme , like our approach.

Another advantage of input space geometric sampling schemes is that they are typically *interpretable*. In contrast, the sampling criterion based on a parametric model tells us which new sample candidate is currently regarded as most informative. When the basis-functions are not trivial, the reason for this rating is a black box that cannot be understood by human.

In the domain of supervised sampling schemes several approaches are model-based but not strictly *optimal*. For example, Cohn (1997) discussed how for a nonparametric approach such as *locally weighted regression* one can sample either to minimize predictive bias or variance. While any combination of both will result in a *robust* sampling scheme, the question was left open how to combine both in order to achieve the true minimization of the joint error components. Another example for this are *Query by committee* approaches, where candidates are scored depending on the disagreement between several models maintained in parallel (see, for example, Seung et al. (1992)).

While supervised sampling schemes are typically at least weakly *optimal* (through a heuristic approximation), they are not necessarily *robust*. For

example, Douak et al. (2013) queries labels where the prediction error is considered largest, which is reasonable under homoscedastic noise assumptions. When accidentally applied in a heteroscedastic scenario, as soon as the true function is coarsely rendered, the sampling process becomes degenerate, as it collapses to the point of largest noise level.

In the following, we will set our focus of the discussion on the one hand to the category of approaches that are *optimal*, *robust* and nonparametric, like our proposed active learning framework. In this category, Goetz et al. (2018) most recently proposed an active learning strategy that is based on purely random trees. On the other hand, we will discuss the wavelet-based approach of Bull et al. (2013), since it provides theoretical guarantees to exceed the minimax-convergence rate of nonparametric active learning approaches that operate on a general function space like  $C^{Q+1}(\mathcal{X})$  (Willett et al., 2006). They achieve this by making use of a more sophisticated segmentation of this very function space, where the segmentation is done with respect to local complexity of the function. Note that the approach of Bull et al. (2013) is not *robust*, as it assumes homoscedastic noise.

## 4.3.1. A random tree/forest active learning approach

Goetz et al. (2018) choose a Mondrian tree  $\hat{f}_{MT}$  as the underlying model of their active learning approach. The tree is first set up by partitioning the input space into cuboids. Then,  $\widehat{f}_{\rm \scriptscriptstyle MT}$  is a constant mean prediction over each such cuboid. Goetz et al. found the following law for the lifetime hyperparameter  $\lambda(n^{1/(2+d)}-1)$  to be optimal. It controls the expected number of splits of the cuboids. As soon as the random tree is set up, there is a model induced bias which is unaffected by the training sample. Accordingly, Goetz et al. minimize the remaining variance for their active learning scheme, which gives an optimal training density  $\hat{p}_{MT}$  that is proportional to the root MSE times test input marginal q on each respective cuboid. Given an initial, randomly chosen training set  $\sim q$ , the criterion can be estimated simply, using the cuboid-wise empirical variances and sample counts. Here, Goetz et al. suggest to set the initial sample size to half the terminal sample size. In the experiments, we will compare to this supervised, nonparemetric active learning approach, since it fulfills the requirements we have imposed in this work: It is optimal and robust, and will likely provide model-agnosticity as well. A single tree is quite a rudimentary model in terms of prediction performance. By setting up a Mondrian forest, that is, an ensemble of random trees where we average their responses, the performance greatly improves. The main shortcoming of a single Mondrian tree is the default prediction, whenever a cuboid contains no training data at all. When combining several

trees, we only need to fall back to the default, when for a test input the associated cuboids of all respective trees are simultaneously empty. Therefore, by increasing the number of trees, we can deploy a larger  $\lambda$  in the law of the lifetime hyperparameter. Regarding active learning, Goetz et al. suggest to sample from  $\hat{p}_{\rm MF}$ , the average of the optimal densities of each individual tree. Note that this heuristic sampling scheme for the Mondrian forest does not preserve theoretical guarantees of optimality.

#### 4.3.2. A wavelet-based approach

It is well known that a nonparametric active learning approach such as ours that operates on a general function space like  $\mathcal{C}^{Q+1}(\mathcal{X})$  is subject to the nonparametric minimax-convergence rate, given by  $O_p\left[n^{-\frac{2(Q+1)}{2(Q+1)+d}}\right]$ , which is already obtained by random test sampling. In particular, it is impossible for nonparametric active learning to increase in rate beyond random test sampling over this function space. Despite this, Bull et al. (2013) have shown that for a more sophisticated segmentation of the function space faster learning rates can be theoretically obtained on adequate subsets of  $\mathcal{C}^{Q+1}(\mathcal{X})$ : Indeed, the model with best, uniform performance over such a subset can exceed the performance of the model that is best over the whole space  $\mathcal{C}^{Q+1}(\mathcal{X})$ . This segmentation is done with respect to local complexity of the function. While they do not come up with an estimate for that enhanced learning rate, they provide an active learning scheme for a wavelet-based prediction model that will asymptotically converge at this rate: The amplitude of wavelet coefficients are used to rank sub-intervals of the input space. Then the training set is refined by deterministically adding samples proportional to the reciprocal of these ranks. Furthermore Bull et al. (2013) state that the subspace of functions for which no increased rate can be obtained is negligible.

Bull et al. assume a homoscedastic noise structure (making it a nonrobust approach) and a uniform test density (leaving it sub-optimal for other test distributions). Also the generalization beyond 1-dimensional input data remains unclear. Yet, the improvement of Bull's approach beyond the minimax-convergence rate that our proposed active learning framework underlies can be a strong advantage over our sampling scheme. We will therefore also compare the work of Bull et al. to our framework in Sec. 5.3 on a dataset of inhomogeneous local function complexity that we adopted from their paper. Our experiment shows that the theoretical rate increase – even though appealing in the asymptotic limit – does not manifest itself in this example at moderate training sizes, which active learning is concerned with. And so, our active learning framework compares favorably Bull's approach in this case.

#### 5. Experiments

In the following experiments we will visualize our theoretical results, compare to approaches from related work and underpin our claim that our active learning scheme preserves its meaningfulness across models. In particular, we compare to a wavelet-based and a random tree based active learning approach, where we adopt for each approach a toy-regression problem on which they are designed to work. By means of a fair comparison, and to demonstrate the *model-agnosticity* of our approach, we will furthermore apply the actively chosen training sets to an *RBF network*, respectively a *random forest* model.

#### 5.1. Measuring the Active Learning Performance

As already mentioned in Sec. 4.3 it is impossible for our active learning scheme to exceed the convergence rate of random test sampling<sup>2</sup>, since LPS is based on the general function space  $C^{Q+1}(\mathcal{X})$ . More precisely, for any fixed training density p with  $\mathbf{X}_n \sim p$ , we know that, according to Theorem 3, there is a constant  $C_Q^p$  with respect to n such that

$$MISE_Q(q|\boldsymbol{X}_n) = \int_{\mathcal{X}} MSE_Q\left(x, \Sigma_Q^n(x)|\boldsymbol{X}_n\right) q(x) dx$$
$$= C_Q^p n^{-\frac{2(Q+1)}{2(Q+1)+d}} (1 + o_p[1]),$$

which holds, in particular, for  $p \equiv q$ .

Yet, we still can benefit from active learning: We can reduce the required sample amount to reach a certain prediction performance by a constant percentage, over random test sampling. For a regression model  $\hat{f}$  that cannot increase in rate, and a training density p, let us define by  $\varrho(\hat{f},p) > 0$  the relative required sample size such that for all large n and  $n' = \varrho(\hat{f},p)n$  we obtain MISE  $(q,\hat{f}|\mathbf{X}_n) \equiv \text{MISE}(q,\hat{f}|\mathbf{X}'_{n'})$ , where  $\mathbf{X}'_{n'} \sim p$  and  $\mathbf{X}_n \sim q$ . The smaller  $\varrho$  is, the better is the training density p. That means, for a reasonable active learning scheme  $\varrho \leq 1$  should hold.

 $<sup>^2 \</sup>rm Recall$  that we have defined  $random \ test \ sampling$  as i.i.d. sampling from the test distribution in Sec. 1.

In the case of LPS, it is  $\rho(\hat{f}_{Opt}^Q, p) = \left[C_Q^p/C_Q^q\right]^{\frac{2(Q+1)+d}{2(Q+1)}}$ . Asymptotically, we can express the ratio as  $C_Q^p/C_Q^q = \text{MISE}_Q\left(q|\mathbf{X}_n'\right)/\text{MISE}_Q\left(q|\mathbf{X}_n\right)$ , such that we can estimate it as the mean error ratio between  $\mathbf{X}_n' \sim p$  and  $\mathbf{X}_n \sim q$  at large, equal training sizes. We then average this estimate over several repetitions.

**Remark 13.** The predictions of the Mondrian tree and forest models are locally constant, and so they share the  $\rho$  of LPS of order Q = 0. That is,

$$\varrho(\hat{f}_{MT},p) = \left[\frac{\textit{MISE}(q,\hat{f}_{MT}|\mathbf{X}_n')}{\textit{MISE}(q,\hat{f}_{MT}|\mathbf{X}_n)}\right]^{\frac{2+d}{2}}, \text{ and } \varrho(\hat{f}_{MF},p) = \left[\frac{\textit{MISE}(q,\hat{f}_{MF}|\mathbf{X}_n)}{\textit{MISE}(q,\hat{f}_{MF}|\mathbf{X}_n)}\right]^{\frac{2+d}{2}}.$$

#### 5.2. Two Dimensional Heteroscedastic Toy-Data

We start with a two-dimensional toy-example, following the experiments of Goetz et al. (2018) in order to show that our approach generalizes to multivariate problems. Furthermore, we compare to the active learning performance of Goetz et al. Note that the approach of Bull et al. (2013) does not naturally generalize to higher dimensions, such that we do not compare with their approach in this first experiment.

All reported values of relative required sample sizes  $\rho$  with respect to random test sampling are calculated as described in Sec. 5.1. Let

$$\begin{split} p(y|x) &= \mathcal{N}(y; f(x), v(x)), \quad \text{where} \\ f(x) &= C \sin\left(2\pi \frac{\|x\|}{\sqrt{d}}\right), \quad \text{and} \quad v(x) = \left\{ \begin{array}{ll} 25, & \forall 1 \leq i \leq d : x_i > 1/d, \\ 1, & \text{else}, \end{array} \right. \end{split}$$

for C = 100,  $x \in \mathcal{X} = [0, 1]^d$  and d = 2. The test inputs  $x \sim q = \mathcal{U}(\mathcal{X})$  are uniformly distributed. An example of the dataset is given to the left in Fig. 2.

First, note that  $f \in \mathcal{C}^{\infty}((0, 1))$ , such that we could apply our approach with arbitrary degree Q. We will delimit our discussion to the cases Q = 1, 3, where we refer to the respective LPS model as local linear smoothing (LLS) for Q = 1 and local cubic smoothing (LCS) for Q = 3. The experimental results are based on 20 repetitions. Applying the Gaussian kernel k, we implement our proposed active learning procedure as described in Sec. 3.5. We start with  $n_0 = 2^{10}$  equidistantly spaced samples and choose the hyperparameters  $\kappa = 2.58, \mathfrak{s} = 1$ , and the constants  $C_v, C_s, C_\sigma, C_\delta$  in order to obtain  $l_{n_0} = 2^6$ ,  $s_{n_0} = 2^{\frac{2}{3}}, \ \underline{\sigma}_{n_0} = 5 \times 10^{-2}$  and  $\delta_{n_0} = 0.1$ . To the left in Fig. 2 we show an example of our noise estimate over the initial training set.



Figure 2: The heteroscedastic experiment: (Left) Exemplary dataset and initial noise estimate at  $n_0 = 2^{10}$ , using (21). Our proposed terminal LOB and optimal training density estimates based on LLS (middle) and LCS (right), using equations (22) and (19).

The proposed optimal sampling densities for LPS of order 1 and 3 are shown in the middle, respectively to the right panel in Fig. 2. The prediction performance over increasing training size can be seen to the left in Fig. 3, where we compare our active sampling scheme to random test sampling. As this figure suggests, we find consistent sample savings within the LPS model class, which we can quantify via estimation of the relative required sample size with respect to random test sampling, as described in Sec. 5.1. We obtain the values  $\varrho(\hat{f}_{\text{Opt}}^1, \hat{p}_{\text{Opt}}^{1,n}) = 0.77 \pm 0.05$  and  $\varrho(\hat{f}_{\text{Opt}}^3, \hat{p}_{\text{Opt}}^{3,n}) = 0.66 \pm 0.07$ , which means that we can save about 23, respectively 34 percent of samples, using the LPS model of order Q = 1 and Q = 3, when sampling according to our proposed optimal density estimate  $\hat{p}_{\text{Opt}}^{Q,n}$  instead of sampling from the test distribution. Hence, in accordance with Theorem 10, this shows the superiority of our proposed active learning framework.

In order to analyze the transferability of our sampling scheme, we now combine our proposed sampling scheme with the Mondrian forest model. As a preconsideration, let us take an isolated look at the Mondrian tree and forest model when applying the active learning approach of Goetz et al.: We found  $\lambda = 2.5$  in the law of the lifetime hyperparameter of the Mondrian tree to work well. As described in Sec. 4.3.1, we draw half of the terminal training size at random from q, from which the optimal density  $\hat{p}_{\rm MT}$  for the tree is estimated. The remaining samples are drawn subsequently in a way



Figure 3: The heteroscedastic experiment: (Left) The median RMSE obtained by LLS and LCS at several training sizes, comparing random test sampling to the respectively proposed optimal sampling. (Right) The RMSE of Mondrian forests under random test sampling, according to the active learning approach  $\hat{p}_{\rm MF}$  of Goetz et al. (2018) and according to the optimal sampling scheme of LLS and LCS. The error bars show the 95% confidence interval.



Figure 4: The heteroscedastic experiment: The terminal training densities by the active learning approach of Goetz et al. (2018), for the Mondrian tree (left) and Mondrian forest (right).

that approaches this density. The average estimated optimal density  $\hat{p}_{\rm MT}$  of the Mondrian tree model can be seen to the left in Fig. 4.  $\hat{p}_{\rm MT}$  is larger, where the noise level is higher, but also in the steep regions of the function f, resulting from the locally constant modelling of the Mondrian tree.

We also implement a Mondrian forest model  $\hat{f}_{\rm MF}$  as described in Sec. 4.3.1 with  $\lambda = 7$  and 100 Mondrian trees. Noting that the prediction performance of the forest increases with the number of trees, the performance has almost converged at 100 trees and computation starts to become intractable by increasing the number further. Goetz et al. propose to use  $\hat{p}_{\rm MF}$ , which is the average  $\hat{p}_{\rm MT}$  over the individual trees of the forest, as the active learning density. Recall that other than  $\hat{p}_{\rm MT}$  for the Mondrian tree being provably optimal, applying  $\hat{p}_{\rm MF}$  for the Mondrian forest is a heuristic.

To the right of Fig. 4 we show the average estimated training density  $\hat{p}_{\rm MF}$  that is associated to the Mondrian forest model. In contrast to the Mondrian tree model, the Mondrian forest shows much lower bias due to the larger


Figure 5: The heteroscedastic experiment: The median RMSE obtained by Mondrian trees  $\hat{f}_{\rm MT}$  and forests  $\hat{f}_{\rm MF}$  at several training sizes, comparing random test sampling to the active learning strategies  $\hat{p}_{\rm MT}$  and  $\hat{p}_{\rm MF}$  of Goetz et al. (2018) for  $\hat{f}_{\rm MT}$ , respectively  $\hat{f}_{\rm MF}$ . The error bars show the 95% confidence interval.

lifetime hyperparameter  $\lambda$ . Therefore the obtained density is mostly driven by the local noise level.

In Fig. 5 we see that the Mondrian tree performance increases significantly with the optimal density  $\hat{p}_{\rm MT}$  of Goetz et al., but the absolute level of the performance of  $\hat{f}_{\rm MT}$  is much lower compared to more sophisticated prediction models, as can be seen in Fig. 3.

When estimating the relative required sample size with respect to random test sampling, we obtain  $\rho(\hat{f}_{\rm MT}, \hat{p}_{\rm MT}) = 0.61 \pm 0.05$  and  $\rho(\hat{f}_{\rm MF}, \hat{p}_{\rm MF}) = 0.90 \pm 0.02$ . The sample savings for the Mondrian tree are substantial, as expected, because  $\hat{p}_{\rm MT}$  is provably optimal for this model. In contrast, the sample savings for the Mondrian forest, although being significant, are much weaker. Recall that  $\hat{p}_{\rm MF}$  was heuristically designed for the Mondrian forest by Goetz et al. And while this heuristic is successful in terms of model transferability, we expect room for further improvement.

Finally, we combine our sampling scheme with the Mondrian forest model. The error curves for the Mondrian forest model in combination with different sampling schemes are shown to the right in Fig. 3.

We observe significant sample savings over random test sampling for the Mondrian forest in combination with our proposed active sampling scheme, with  $\varrho(\hat{f}_{\rm MF}, \hat{p}_{\rm Opt}^{1,n}) = 0.68 \pm 0.02$  and  $\varrho(\hat{f}_{\rm MF}, \hat{p}_{\rm Opt}^{3,n}) = 0.62 \pm 0.02$  for our proposed optimal training density estimates with Q = 1, respectively Q = 3. This first of all provides evidence that our proposed active sampling scheme is model-agnostic.

Furthermore, recalling that it was  $\rho(\hat{f}_{\rm MF}, \hat{p}_{\rm MF}) = 0.90 \pm 0.02$ , both values beat the active learning performance of  $\hat{p}_{\rm MF}$  by far. In fact, we can save about 24, respectively 31 percent of samples when applying our active learning framework with Q = 1 and Q = 3 instead of  $\hat{p}_{\rm MF}$ , which was specifically crafted for the Mondrian forest.



Figure 6: The Doppler experiment: (Left) Exemplary dataset. (Right) Asymptotic and estimated locally optimal bandwidths, using equations (15) and (22).

#### 5.3. Doppler Function

As described in Sec. 4.3.2, the wavelet-based approach by Bull et al. (2013) is designed to adapt to inhomogeneous complexity under homoscedastic noise  $v(x) \equiv v$ , assuming a uniform test density  $q \sim \mathcal{U}(\mathcal{X})$ . In theory, their approach is asymptotically capable of exceeding the convergence rate of our proposed active learning framework, which is why we will compare both, qualitatively and quantitatively. We will also include the Mondrian forest approach of Goetz et al. (2018) from the first experiment, noting that it is not a promising candidate for a dataset of inhomogeneous complexity: The Mondrian forest model has no adaption parameter in the sense of local bandwidth, as opposed to the wavelet and our approach.

Bull et al. used the Doppler function (see, for example, Donoho and Johnstone (1994)) as a prototype where they expect such an increase in rate due to the strong inhomogeneous complexity of the function to learn. We adopt their experimental specification: For  $x \in \mathcal{X} = [0, 1]$ , let

$$p(y|x) = \mathcal{N}(y; f(x), 1), \quad f(x) = C\sqrt{x(1-x)}\sin(2\pi(1+\epsilon)/(x+\epsilon)),$$

where  $\epsilon = 0.05$ , C is chosen such that  $||f||_2 = 7$  and  $\mathcal{N}(\cdot; \mu, \sigma^2)$  denotes the Gaussian distribution with mean  $\mu$  and variance  $\sigma^2$ . Fig. 6 (Left) shows an example dataset. In this experiment we know that  $q \sim \mathcal{U}(\mathcal{X})$  and the problem is homoscedastic. Applying the Gaussian kernel k, we implement our proposed active learning procedure as described in Sec. 3.5. We start with  $n_0 = 2^9$  equidistantly spaced samples and choose the hyperparameters  $\kappa = 1.96, \mathfrak{s} = 2$ , and the constants  $C_s, C_\sigma, C_\delta$  in order to obtain  $s_{n_0} = 2^{\frac{2}{3}}$ ,  $\underline{\sigma}_{n_0} = 1.5 \times 10^{-3}$  and  $\delta_{n_0} = 0.1$ . An example of our LOB estimate for Q = 1 is given to the right in Fig. 6.

While again  $f \in \mathcal{C}^{\infty}((0, 1))$ , we will delimit our discussion to the cases Q = 1, 3. The experimental results are based on 30 repetitions. In Fig. 7 we



Figure 7: The Doppler experiment: (Left) The optimal training density estimates of our approach for the polynomial degrees Q = 1, 3 at training size  $n = 2^{15}$ . The median maximal absolute error (middle) and RMSE (right) obtained by LPS with the respective active sampling scheme and random test sampling ( $\sim q$ ) at various training sizes. The error bars show the 95% confidence interval.



Figure 8: The Doppler experiment: (Left) The terminal training density of Goetz' (red), Bull's (purple) and our approach (blue). The median maximal absolute error (middle), respectively RMSE (right) obtained by Goetz', Bull's and our model with the respective active sampling scheme and random test sampling ( $\sim q$ ) at various training sizes. The error bars show the 95% confidence interval.

show the achieved performance of both cases, when either sampling from the test distribution  $\sim q$ , or when sampling according to the respective optimal training density estimate, which is plotted to the left.

Like in the first experiment, we calculate the relative required sample size with respect to random test sampling, as described in Sec. 5.1. Again, confirming our result in Theorem 10, we observe significant sample savings of  $\rho(\hat{f}_{\text{Opt}}^1, \hat{p}_{\text{Opt}}^{1,n}) = 0.64 \pm 0.02$  and  $\rho(\hat{f}_{\text{Opt}}^3, \hat{p}_{\text{Opt}}^{3,n}) = 0.53 \pm 0.03$ .

For a comparison to the active sampling approach of Bull et al., we implement their method in *python*, based on the *pywt* package, and using the Daubechies-wavelets of filter length 8 (DB8). The resulting training density can be seen to the left in Fig. 8, together with the densities of Goetz' and our approach. We observe that all approaches spend more samples to the left – as expected – where Bull's and our approach concentrate the more samples,

the higher the local function complexity becomes. Here, the density of Bull's approach increases steeper to the left of the input space.

Furthermore, we observe to the middle and right of Fig. 8 that the LPS model class shows better performance than the wavelet-based approach, especially at smaller samples size. At sample size  $2^{12}$  the wavelet-based approach allows for enough flexibility to adapt locally, which leads to the sudden dissociation of the learning curves of the wavelet-based approach under Bull's sampling scheme compared to *random test sampling* in Fig. 8. After that, both approaches follow almost parallel learning curves. This indicates that, in practice, there are regression problems where the theoretically achievable enhancement of the learning rate (with a function space segmentation such as in Bull et al.) is negligible. While it is theoretically appealing to achieve a better learning rate in the asymptotic limit, active learning is usually concerned with small to moderate sample sizes. In this regime, a constant percentage of sample savings, as achieved by our approach, can be of greater benefit.

Note that the actual RMSE decay law of the wavelet-based model is unknown. Yet, since the RMSE of the wavelet approach decays at least as fast as for LCS, we can upper bound the active learning performance of Bull's approach by calculating the relative required sample size with respect to random test sampling analogously to  $\varrho(\hat{f}_{Opt}^3, \hat{p}_{Opt}^{3,n})$ , which gives  $\varrho(\hat{f}_{Bull}, \hat{p}_{Bull}) = 0.82 \pm 0.03$ . Thus, we can say that we save about 47 percent of samples with our active learning framework compared to random test sampling on the LCS model, whereas we save at most 18 percent with Bull's active learning approach on the wavelet-based model.

Since both models are not directly comparable, we cannot deduce from these numbers which sampling scheme is better. In this regard, we will adopt a radial basis function network as a regression model from the domain of neural network learning, for which both active learning approaches are not optimized. We will train the RBF-network, using *random test sampling*, as well as the actively chosen training sets of Bull's, Goetz' and our approach. In addition, we assume a small validation dataset of size  $2^{10}$  to be given. A successful outcome first of all underpins the claimed *model-agnosticity* of our proposed active learning framework. Second, it allows for a fair comparison of the three approaches.

The RBF-network (Moody and Darken, 1989) is implemented in *PyTorch* (Paszke et al., 2019) with a few hyperparameters: Its RBF-layer consist of N Gaussian basis function nodes with bandwidths  $\sigma_i$  and centers  $\mu_i$ , followed



Figure 9: The Doppler experiment: The median RMSE obtained by a radial basis function network  $\hat{f}_{\rm NN}$  at several training sizes, when trained with *random test sampling*, respectively Bull's, Goetz' and our proposed active sampling scheme. The error bars show the 95% confidence interval.

by a linear layer with weights w. Formally,

$$\widehat{f}_{NN}(x) = w_0 + \sum_{i=1}^N w_i k^{\sigma_i}(\mu_i, x).$$

The RBF-nodes are initialized with  $\sigma_i = \sigma_0 \left(\frac{n}{n_0}\right)^{-\frac{1}{5}}$ , and centers  $\mu_i$  (sub-)sampled from the current training dataset.

We apply the training MSE as the training objective. In addition, inspired by Lepski's method, we favor larger local bandwidths over smaller ones when they perform similarly. Therefore we add the term  $-\lambda \sum_{i=1}^{N} \log\{\sigma_i\}$  to the objective to penalize small bandwidth choices, where we set the penalty factor  $\lambda = \lambda_0 \frac{N}{2^9} \left(\frac{n}{n_0}\right)^{-\frac{1}{2}}$ . The training is then done, using the AdamW-optimizer (Loshchilov and Hutter, 2018) with a weight decay of  $\nu_0 \left(\frac{n}{n_0}\right)^{-\frac{1}{2}}$  and minibatches of the training data of size  $B = \lceil B_0 \left(\frac{n}{n_0}\right)^{\frac{1}{2}} \rceil$ . We initialize a shared learning rate factor of  $l = 10^{-2}$  that we gradually decrease towards  $10^{-7}$ whenever the validation error gets stuck. Using this shared learning rate factor, we apply individual initial learning rates for the linear weights  $l_w = l$ , the bandwidths  $l_{\sigma} = 0.5l$  and the centers  $l_{\mu} = 0.1l$ .

For all sampling schemes we apply the same set of hyperparameters  $B_0 = 4$ ,  $\sigma_0 = 7 \times 10^{-4}$ ,  $\lambda_0 = 1.6$  and  $\nu_0 = 8 \times 10^{-3}$ , where we only choose the number of RBF-nodes N individually: For Bull's as well as our approach,  $N = 2^9$  works best, whereas for all other approaches  $N = 2^{11}$  works best. The heavy local complexity towards zero is only recognized properly by Bull's and our approach such that the number of RBF-node centers near zero is large enough at this smaller total number of nodes.

In Fig. 9 we observe that all approaches, Bull's, Goetz' and ours, outper-

form random test sampling for the RBF-network model  $\hat{f}_{\rm NN}$ . This first of all underpins the transferability of all these sampling schemes. To the left in Fig. 8 we have seen that Bull's and our sampling scheme act qualitatively similar on this dataset. Therefore, as expected, both approaches also behave quantitatively similar. For an exact quantitative analysis, note that the MISE of the RBF-network model follows the decay law  $\sim n^{-1}$ . Accordingly, we can calculate the required sample size relative to random test sampling, for which we obtain the values  $\rho(\hat{f}_{\rm NN}, \hat{p}_{\rm MF}) = 0.79 \pm 0.05$ ,  $\rho(\hat{f}_{\rm NN}, p_{\rm Bull}) = 0.62 \pm 0.05$ and  $\rho(\hat{f}_{\rm NN}, \hat{p}_{\rm Opt}^{3,n}) = 0.61 \pm 0.04$ . Thus, Bull's and our approach are significantly better than Goetz' approach in terms of transferability on this dataset. Furthermore, our sampling scheme compares favorably but not significantly to Bull's sampling scheme.

### 5.4. Discussion

We have chosen the toy-examples above from the domain of regression problems, for which the approach of Goetz et al., respectively Bull et al. is designed to work. Since these approaches and our active learning framework are *model-agnostic*, it is not surprising that all resulting sampling schemes behave qualitatively similar. Yet, we obtained equal or better across-model performance with our proposed sampling scheme. Additionally, our approach is more flexible, regarding the applicable class of regression problems: The approach of Bull et al. assumes a uniform test distribution and homoscedastic noise, and it lacks a straight-forward extension to multivariate problems (d > 1). Goetz' approach has degrading performance for inhomogeneously complex regression problems, since its underlying model features no local adaptivity parameter such as LOB. In contrast, our active learning framework does not suffer from these limitations, but incorporates these properties in the optimal sampling scheme instead.

As we have already discussed in Sec. 4.3.2, Bull's sampling scheme may feature an MISE decay law superior to our approach. Hence, asymptotically it should exceed the performance of our approach. But the experiment suggests that this will not occur at reasonable training sizes. The advantage of Goetz' approach is that the model class of random trees is better suited for high-dimensional multivariate problems – a property that the implementation of our theory lacks: In this paper, we construct the optimal training density from pointwise estimators of LOB and the noise level. In future work, this can be remedied by modelling these components as functions.

#### 6. Conclusion and Outlook

The goal of our work was to reconcile the advantages of model-free active learning approaches in regression such as *robustness* and *model-agnosticity*, with the advantages of model-based active learning approaches such as *optimality*. An active sampling scheme with these properties is ideal to construct a larger training set, when we face a regression problem for which the stateof-the-art is still evolving due to, for example, scarce domain knowledge.

As an ansatz to achieve this goal, we consider local polynomial smoothing (LPS), a nonparametric model class with minimal assumptions on the labels, which can be regarded as almost model-free. In terms of locally optimal bandwidths, we chose the mean integrated squared error of LPS as our objective, which we aim to minimize with respect to the training dataset. Making use of the asymptotic behavior of the objective, as well as the isotropic optimal bandwidths, the optimization could be shown to be analytically solvable. The result is obtained in closed-form in terms of the optimal training density  $p_{Opt}^{Q,n}$ , which nicely factorizes the influence of problem intrinsic properties on the optimal sample demand, that is, local function complexity, noise variance and test relevance. This makes our sampling scheme transparent and *interpretable*, a desired property in critical real-world applications. Additionally, the sampling process  $X_n^* \sim p_{Opt}^{Q,n}$  is *stationary*, which enables batch sampling and is advantageous when on demand label annotation is a bottleneck.

Using Lepski's method for the estimation of isotropic, locally optimal bandwidths, we derived a practical implementation of our theory. In experiments, we then compared to related work. Furthermore, we provided evidence that our proposed sampling scheme is *model-agnostic* by applying our actively sampled training data to other model classes. In particular, we observed a consistent performance increase over *random test sampling* for a radial basis function network and a Mondrian forest model. Moreover our active learning framework compared favorably to state-of-the-art nonparametric active learning approaches.

One possible way of generalizing our theory is to consider a non-isotropic candidate set  $S \subseteq \mathbb{S}_{++}^d$ , over which we build our objective (3). A straightforward extension of the proof of our theory from the isotropic case would require the existence of an explicit asymptotic form of LOB. While this existence can be guaranteed under mild assumptions in the isotropic case, it can not in the non-isotropic case – as we have indicated in the beginning of Sec. 2: In particular, the crucial assumption is that the leading terms of bias and variance – as, for example, given in Theorem 3 – do not vanish, almost everywhere. In the general bandwidth case with Q = 1 however, this

only holds if we require f to be indefinite at most on a set of measure zero, which we will call the *definiteness assumption*. This definiteness assumption is a tremendous restriction on f, which most multivariate functions will not fulfill.

When dropping the definiteness assumption,  $\Sigma_Q^n$  from (5) is not welldefined and, even if we find a minimizing bandwidth  $\Sigma_x$  as in (2), the theory on its asymptotics is not elaborated, yet. We discuss these issues that do arise in the general bandwidth case, when in particular not relying on the definiteness assumption, and provide solutions that still make our theory hold in Appendix B.

In particular, we prove the existence of  $\Sigma_x$  as in (2) under mild conditions, and analyze its asymptotic scaling behavior, which depends on the smoothness of f in x. Here, we also constructed a minimal, controlled 2-dimensional toy-example with local *anisotropic* bandwidths to substantiate our theory on the asymptotic behavior of non-isotropic LOB. While we can not guarantee the uniqueness of such an optimal bandwidth, we will show that  $|h_n^{-1}\Sigma_x|^{-1}$  is asymptotically unique, where  $h_n$  is the appropriate bandwidth decay rate in x, as the training size n grows. From this point, a straightforward generalization of Definition 9 to a definition of non-isotropic LFC as in Definition 9 emerges, and an again straightforward generalization of the optimal training density (19) in Theorem 10 becomes apparent.

Unfortunately, in lack of an estimate to LOB in the non-isotropic bandwidth case, we cannot apply our proposed active learning framework in practice at this point. Yet, we would like to emphasize that our framework can readily be applied, once such an estimate becomes available.

Other future work will dedicate a practical application of our novel framework for domains like quantum chemistry or materials properties, where data is extremely expensive (e.g. Butler et al. (2018); von Lilienfeld et al. (2020); Keith et al. (2021)).

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# Appendix A. Nomenclature

### Variables

X	The input space, being a subset of $\mathbb{R}^d$
S	The bandwidth candidate space with $\mathcal{S} \subseteq \mathbb{S}^d_{++}$
d	The dimension of the input space $\mathcal{X}$
Q	The polynomial order of the LPS model
k	The RBF-kernel function
f	The regression function to infer
v	The local noise variance function
p	The density of the training input distribution
q	The density of the test input distribution
$\alpha = L + \beta$	The Hölder exponent with $L \in \mathbb{N}$ and $\beta \in (0, 1]$
$\varrho$	The relative required sample size with respect to $random \ test$
	sampling

# Operations

$\left M ight ,\left A ight $	The determinant of a square matrix $M \in \mathbb{R}^{d \times d}$ or the cardinality
	of a set $A$
$A^{\circ}$	The interior of a metric set $A$
$M^{ op}$	The transpose of a matrix $M \in \mathbb{R}^{m \times n}$
trace(M)	The trace of a matrix $M \in \mathbb{R}^{m \times n}$
$\mathbf{vec}(A)$	The arbitrarily, but fixed ordered vectorization of a finite set $A$
$\mathbb{1}_d$	The vector of ones in $\mathbb{R}^d$
diag(v)	The diagonal matrix with the entries of the vector $v$ on its diagonal
$\mathcal{I}_d$	The identity matrix $diag(\mathbb{1}_d) \in \mathbb{R}^{d \times d}$
$\mathbb{E} Z$	The expectation of a random variable $Z$
$\mathbb B$	The bias function
V	The variance function
$\mathcal{U}(A)$	The uniform distribution over a set $A$ of finite measure
$\mathcal{N}(\cdot;\mu,\sigma^2)$	The Gaussian distribution with mean $\mu$ and variance $\sigma^2$
$D_f^l(x)$	The tensor of <i>l</i> -th order partial derivatives of $f$ in $x \in A$ for
5	$f\in\mathcal{C}^{l}\left(A\right)$
$\mathbb{1}_A(x)$	The indicator function, returning 1 for $x \in A$ and 0, else
sgn(x)	The sign function $2 \cdot 1_{\mathbb{R}_+}(x) - 1$

## Sets

The natural numbers
The real, nonnegative real and positive real numbers
The space of symmetric matrices $M \in \mathbb{R}^{d \times d}$ with $M^{\top} = M$
The space of positive definite matrices $M \in \mathbb{S}^d$ with $a^{\top}Ma > a$
$0, \forall a \in \mathbb{R}^d \setminus \{0\}$
The space of real polynomial mappings $\mathfrak{p} \colon \mathbb{R}^d \to \mathbb{R}$ up to order $Q$
The space of c-times differentiable mappings $f: A \to B$
The shorthand for $\mathcal{C}^{c}(A,\mathbb{R})$
The space of probability step-functions on the set $A$
The space of random sequences $X_n$ that converge strictly faster,
respectively strictly slower or at equal rate in probability to 0,
compared to $a_n$
The space of random sequences $X_n$ that are upper, respectively
lower bounded in probability by $a_n$

## Acronyms

LPS	Local polynomial smoothing
LLS	Local linear smoothing
LCS	Local cubic smoothing
MSE	Mean squared error
RMSE	Root mean squared error
MISE	Mean integrated squared error
MAE	Maximum absolute error
LOB	Locally optimal bandwidth
LFC	Local function complexity
$\operatorname{RBF}$	Radial basis function
GPR	Gaussian process regression

### Constants

$C_v$	The factor of the noise estimate localization
$C_s$	The constant in the adaptive bandwidth step size in Lepski's method
$C_{\sigma}$	The constant in the adaptive smallest bandwidth in Lepski's method
$C_{\delta}$	The constant in the adaptive radius for the stabilization of local
	estimates
$\kappa$	The confidence interval size factor in Lepski's method
5	The standard deviations factor of the kernel for boundary correction

### Appendix B. Analysis of the Non-isotropic Case

In the first part of this paper we discussed the space of isotropic bandwidth, where we could derive our optimal sampling theory in a simplified way: Due to LOB being well-defined in this case, it exhibits an asymptotic closedform from which the balancing property as well as its asymptotic scaling immediately followed. Also the literature on LOB mostly concentrates on the isotropic bandwidth case for practical reasons: It is not straight-forward to come up with an estimate to non-isotropic LOB. Yet, in case that future research comes up with estimates to non-isotropic LOB, we would like to analyze in advance to what extent the asymptotic theory on LOB, LFC and optimal sampling will generalize.

In summary, we will find out that under reasonable assumptions LOB also exists in the non-isotropic case, but the resulting MSE will generally decay at a substantially different law. Here, LOB is not necessarily unique, and hence may not exhibit an asymptotic closed-form. Fortunately, the determinant of LOB is unique, which enables a straight-forward generalization of isotropic LFC, as given in Definition 9, under some restrictions on the training distribution. Finally, due to the restrictions on the training distribution, we are not able to solve for the optimal training density analytically. However, we can formulate a closed-form heuristic, which is the straight-forward looking generalization of the optimal training density in the isotropic case.

From here on, we assume a non-isotropic bandwidth candidate space  $S \subseteq \mathbb{S}_{++}^d$ , where d > 1 as the notion of non-isotropy makes no sense in the 1-dimensional case. Furthermore, we assume a symmetric kernel k, and, for convenience, we restrict ourselves to the well-known local linear smoothing (LLS) model, that is, LPS of order Q = 1, noting that the extension to an arbitrary order of the LPS model is straight-forward.

**Remark B1.** If not explicitly stated differently, we discuss the case  $S = \mathbb{S}_{++}^d$ , noting that several results may hold true, when considering true subsets  $S \neq \mathbb{S}_{++}^d$  that are conic. In particular S is conic, if  $S = \bigcup_{\Sigma \in S} \bigcup_{a \in \mathbb{R}_+} \{a\Sigma\}$ .

### Appendix B.1. Non-isotropic Locally Optimal Bandwidths

The key difference we have to treat is, whether or not the leading bias term of order (Q + 1) can be canceled a.e. over the input space for an appropriate local choice of bandwidth matrix. In the case of LLS and  $S = \mathbb{S}_{++}^d$  the question above simplifies to whether f fulfills the definiteness assumption, mentioned in the introduction. This can be understood by taking a look at the bias-variance-decomposition: Let  $\mu_2 = \int u^2 k(u) du$  and  $R(k) = \int k^2(u) du$ . When holding  $\Sigma \in \mathbb{S}_{++}^d$  fixed, the asymptotic form of the leading bias- and variance-terms is known:

**Theorem B2** (Ruppert and Wand (1994)). Let  $h_n \to 0$ ,  $nh_n^d \to \infty$  as  $n \to \infty$ and  $x \in \mathcal{X}^\circ$  with p(x) > 0. Furthermore let  $f \in \mathcal{C}^2(\mathcal{X})$  with Hessian  $D_f^2(x)$ ,  $p \in \mathcal{C}^1(\mathcal{X})$  and  $v \in \mathcal{C}^0(\mathcal{X})$ . Then, for a fixed  $\Sigma \in \mathbb{S}^d_{++}$ , it is

$$\mathbb{B}_{1}\left[x,h_{n}\boldsymbol{\Sigma}|\boldsymbol{X}_{n}\right]=bias_{1,2}\left[x,h_{n}\boldsymbol{\Sigma}\right]+o_{p}\left[h_{n}^{2}\right]$$

and

$$\mathbb{V}_{1}\left[x, h_{n} \Sigma | \boldsymbol{X}_{n}\right] = var_{1}\left[x, h_{n} \Sigma | \boldsymbol{X}_{n}\right] + o_{p}\left[n^{-1} h_{n}^{-d}\right],$$

where for  $Z \in \mathbb{S}^d_{++}$  we define

$$bias_{1,2}[x,Z] = \frac{1}{2}\mu_2 trace(D_f^2(x)Z^2),$$
 (B.1)

$$var_1[x, Z | \boldsymbol{X}_n] = \frac{R(k)v(x)}{|Z|\,p(x)n}.$$
(B.2)

Therefore the conditional mean squared error in x can be expressed as

$$MSE_{1}[x, h_{n}\Sigma|\boldsymbol{X}_{n}] = bias_{1,2}[x, h_{n}\Sigma]^{2} + var_{1}[x, h_{n}\Sigma|\boldsymbol{X}_{n}] + o_{p}[h_{n}^{4} + n^{-1}h_{n}^{-d}]$$

**Remark B3.** For  $\Sigma = \mathcal{I}_d$ , both formulations, (13), (14) and (B.1), (B.2) of asymptotic bias and variance coincide. In this sense, Theorem B2 is a generalization of Theorem 3 for (Q = 1).

Now, if f fulfills the definiteness assumption, then LOB exists uniquely and exhibits a closed-form asymptotic solution:

**Corollary B4** (Fan et al. (1997)). May the conditions of Theorem B2 hold and assume that  $p(x), v(x) \neq 0$  and f is definite in x. When searching for LOB in the space of positive definite bandwidth candidates  $S = \mathbb{S}^d_{++}$ , asymptotically it is

$$\Sigma_{1,\mathbb{S}_{++}^d}^n(x) = \Sigma_{Asymp}^{1,n}(x) + o_p \left[ n^{-\frac{1}{4+d}} \right], \quad for$$
  
$$\Sigma_{Asymp}^{1,n}(x) = \left[ \frac{R(k)v(x) \left| \sqrt{D_f^2(x)^+} \right|}{p(x)n\mu_2^2 d} \right]^{\frac{1}{4+d}} \sqrt{D_f^2(x)^+}^{-1}, \qquad (B.3)$$

where  $D_f^2(x)^+ = \begin{cases} D_f^2(x), & \text{if } D_f^2(x) \text{ is positive definite} \\ -D_f^2(x), & \text{if } D_f^2(x) \text{ is negative definite}, \end{cases}$ and  $\sqrt{\Sigma} \in \mathbb{S}_{++}^d$  such that  $\sqrt{\Sigma} \cdot \sqrt{\Sigma} = \Sigma$  for  $\Sigma \in \mathbb{S}_{++}^d$ . Therefore, in the case of (Q = 1) and almost everywhere definite f, Corollary B4 generalizes Corollary 6 to the positive definite bandwidth candidate space. It is noteworthy that in this case we do not benefit from fbeing smoother than  $C^2$  up to a constant factor. In particular there is no rate increase, using non-isotropic over isotropic LOB.

In contrast, if f does not fulfill the definiteness assumption, we can show that LOB still exists under weaker conditions. In this case, the asymptotics of LOB and the associated MSE behaves surprisingly different. We refer to Appendix E for a detailed derivation.

In preparation for this, we need to notion of consistent sequences

$$\mathfrak{S} = \left\{ (\Sigma^n)_{n \in \mathbb{N}} \subset \mathcal{S} \left| \left| \Sigma^n \right|^{-1} n^{-1} \to 0, \left\| \Sigma^n \right\| \to 0, \left\| \Sigma^n \right\| \cdot \left\| [\Sigma^n]^{-1} \right\| \le \mathcal{M} \right\},$$
(B.4)

where  $\mathcal{M} < \infty$  is an arbitrary constant. We further need to define the pointwise Hölder smoothness of f:

**Definition B5.** The function f belongs to the pointwise Hölder space  $\Lambda^{\alpha}(x)$ , if for  $\alpha = Q + \beta$  with  $Q \in \mathbb{N}$  and  $\beta \in (0, 1]$  there exists a constant  $C_x > 0$ , a closed ball  $\overline{B}_{\delta_x}(x) = \{x' \in \mathbb{R}^d \mid ||x - x'|| \leq \delta_x\} \subset \mathcal{X}$  for some  $\delta_x > 0$  and a polynomial  $P \in \mathcal{P}_Q(\mathbb{R}^d)$  such that

$$\sup\left\{\left|f(x') - P(x)\right| \le C_x \|x - x'\|^{\alpha} \mid x' \in \bar{B}_{\delta_x}(x)\right\}.$$

The pointwise Hölder exponent of f in x is then given by

$$\alpha(f, x) = \sup \left\{ a > 0 \mid f \in \Lambda^a(x) \right\}.$$

**Remark B6.** If  $f \in C^{\alpha}(\mathcal{X})$ , then  $f \in \Lambda^{\alpha}(x)$  such that  $\alpha(f, x) \geq \alpha$  for all  $x \in \mathcal{X}$ .

With these two definitions, we are able to state the following result (see Appendix E):

**Theorem B7** (Non-isotropic LOB and MSE of LLS for indefinite functions). Let  $S = \mathbb{S}_{++}^d$  with  $d \ge 2$ . Let  $x \in \mathcal{X}^\circ$  where for  $\alpha := \alpha(f, x)$  it holds that  $2 < \alpha < \infty$  and write  $\alpha = L + \beta$  with  $L \in \mathbb{N}, L \ge 2$  and  $\beta \in (0, 1]$ . Furthermore assume that  $k \in C^{\lfloor L/2 \rfloor}(\mathbb{R}_+, \mathbb{R}_+)$ , v is continuous in x and  $p \in \Lambda^{\alpha-2}(x)$  with p(x), v(x) > 0. If f is indefinite in x, then there exists a sequence  $(\Sigma_x^n)_{n\in\mathbb{N}} \in \mathfrak{S}$  such that with  $h_n = n^{-\frac{1}{2\alpha+d}}$ ,

$$MSE_1\left(x, \Sigma_x^n | \boldsymbol{X}_n\right) = \theta_p \left[h_n^{2\alpha}\right] = \theta_p \left[n^{-\frac{2\alpha}{2\alpha+d}}\right],$$

and  $N_x \in \mathbb{N}$  such that for all  $(\Sigma^n)_{n \in \mathbb{N}} \in \mathfrak{S}$ , if  $n \geq N_x$ , it holds that

$$MSE_1(x, \Sigma_x^n | \mathbf{X}_n) \le MSE_1(x, \Sigma^n | \mathbf{X}_n)$$

For such a sequence,  $\Sigma_x^n = \theta_p \left[ n^{-\frac{1}{2\alpha+d}} \mathbb{1}_d \mathbb{1}_d^\top \right]$  and  $\inf_{\Sigma \in \mathcal{T}_1^x} \|h_n^{-1} \Sigma_x^n - \Sigma\| = O_p \left[h_n^2\right]$  must hold.

The intuition behind the above theorem is as follows: By assumption, we are able to strictly eliminate the bias of (the slowest) second order. Accordingly let  $\Sigma \in \mathcal{S}$  be such a root. Due to the  $\alpha$ -smoothness of f in x, we can explicitly expand the bias to the order of the next smaller integer (see Appendix C). Now we can perturb  $\Sigma$  in such a way that the second-order bias-term equals minus the sum of the remaining higher-order bias-terms. It remains a bias of the order  $O_p\left[||\Sigma||^{\alpha}\right]$  that cannot be eliminated. In Appendix D, we demonstrate this phenomenon in a controlled 2-dimensional toy-example.

While we now know about the existence of LOB in the indefinite regime, we know nothing about its uniqueness. In particular, we have no explicit asymptotic form, like in the definite case. We may still define the set-valued function of minimizers

$$\Sigma_{1,\mathcal{S}}^{n}(x) = \left\{ \Sigma \in S_{n} \mid \mathrm{MSE}_{1}\left(x, \Sigma | \boldsymbol{X}_{n}\right) = \min_{\Sigma' \in S_{n}} \mathrm{MSE}_{1}\left(x, \Sigma' | \boldsymbol{X}_{n}\right) \right\}, \quad (\mathrm{B.5})$$

where we delimit the bandwidth search space reasonably, as in the proof of Lemma E3, by

$$S_n = \left\{ \Sigma \in \mathcal{S} \mid \|\Sigma\| \le n^{-\gamma}, |\Sigma| \ge n^{-1} \right\},\$$

using  $\gamma = \frac{1}{2\alpha + d + 1}$  to exclude inconsistent solutions.

Appendix B.2. Non-isotropic Local Function Complexity

Let us first take a look at the definite case: Here, we know from Corollary B4 about the asymptotic scaling of LOB. Hence, a straight-forward generalization of LFC from the isotropic case in Definition 9 is given as follows:

**Definition B8** (Non-Isotropic LFC of LLS in the definite case).

For  $S = \mathbb{S}^d_{++}$ , let  $\Sigma^n_{1,\mathbb{S}^d_{++}}$  be the optimal bandwidth function as defined in (B.5). For f definite in x, we define by

$$\mathfrak{C}^{n}_{1,\mathbb{S}^{d}_{++}}(x) = C^{d}_{1} \Big[ \frac{v(x)}{p(x)n} \Big]^{\frac{d}{4+d}} \left| \Sigma^{n}_{1,\mathbb{S}^{d}_{++}}(x) \right|^{-1}$$
(B.6)

the LFC of f in x with respect to the LLS model.

Like in the isotropic case,  $\mathfrak{C}^n_{1,\mathbb{S}^{d}_{++}}$  is asymptotically continuous and independent of the global scaling with respect to training size n, as well as the local scaling with respect to the training density p and noise level v, which can be seen by writing

$$\mathfrak{C}_{1,\mathbb{S}_{++}^{d}}^{n}(x) = \mathfrak{C}_{1,\mathbb{S}_{++}^{d}}^{\infty}(x)(1+o_{p}[1]), \text{ where}$$
$$\mathfrak{C}_{1,\mathbb{S}_{++}^{d}}^{\infty}(x) = \left[\frac{\mu_{2}d}{2}\right]^{\frac{2d}{4+d}} \left|\sqrt{D_{f}^{2}(x)^{+}}\right|^{\frac{4}{4+d}}.$$
(B.7)

**Remark B9.** The isotropic and the generalized definitions of LFC in (17) and (B.6) coincide asymptotically, if an isotropic bandwidth is, in fact, the optimal solution to the generalized case. That is, if we can write  $D_f^2(x) = g(x)\mathcal{I}_d$  for some scalar-valued function g, then

$$\begin{split} \mathfrak{C}_{1,\mathbb{S}_{++}^d}^{\infty}(x) &\stackrel{(\mathrm{B.7})}{=} \left[\frac{\mu_2 d}{2}\right]^{\frac{2d}{4+d}} |g(x)|^{\frac{2d}{4+d}} = \left[\frac{\mu_2}{2} \operatorname{trace}\{D_f^2(x)\}\right]^{\frac{2d}{4+d}} \\ &\stackrel{(\mathrm{B.1})}{=} \operatorname{bias}_1[x,\mathcal{I}_d]^{\frac{2d}{4+d}} \stackrel{(\mathrm{18})}{=} \mathfrak{C}_1^{\infty}(x). \end{split}$$

When moving on to the indefinite case, we struggle to define LFC as a function of  $\sum_{1,\mathbb{S}_{++}^d}^n$  on first glance, because LOB is not necessarily a proper function over the input space. Fortunately, we can show the following (see Appendix F):

**Theorem B10.** Let  $f \in C^{\alpha}(\mathcal{X})$  and may the assumptions of Theorem B7 hold uniformly with  $\alpha(f, x) \equiv \alpha$  for all  $x \in \mathcal{X}^{\circ}$ . Then there exist  $D_n \in C^0(\mathcal{X}, \mathbb{R}_{++})$  such that

$$\left|h_n^{-1} \Sigma_{1,\mathbb{S}_{++}^d}^n(x)\right|^{-1} = D_n(x) + o_p[1],$$

almost everywhere in  $\mathcal{X}$ . Furthermore there exists a limiting function D such that

$$D_n(x) = D(x) + o_p \left[1\right].$$

In particular this means that, if  $\Sigma_n, \Sigma'_n \in \Sigma_{1,S_{++}^d}^n(x)$  are both optimal for prediction in x, then they asymptotically share their reciprocal determinant. For finite n the reciprocal determinant is close to a continuous function over the input space. Finally, the reciprocal determinant is itself pointwise convergent as  $n \to \infty$ , which enables an asymptotic analysis:

We know that, whether f is definite or indefinite has no influence on the asymptotic variance as defined in (B.2). On the other hand, the bias will behave substantially different. And even though we have no access to an explicit form, we expect it to depend on p and its derivatives, since the explicit higher-order bias-terms do so. All we can say is, that the bias will not depend on v and n.

We can partially remedy the above problem by enforcing p to have vanishing derivatives, almost everywhere. In particular, let us define the set of probability step-functions:

**Definition B11.** We call  $p \in \mathfrak{P}(\mathcal{X})$  a probability step-function if p is a probability density over  $\mathcal{X}$ , and there exists a finite partition  $\mathcal{X} = X_1 \uplus \ldots \uplus X_S$  of the input space with constants  $P_1, \ldots, P_S > 0$  such that

$$p(x) = \sum_{s=1}^{S} \mathbb{1}_{X_s}(x) P_s.$$

Then we obtain the following result of LFC in the indefinite case:

**Definition B12** (Non-isotropic LFC of LLS in the indefinite case). May the assumptions of Theorem B7 hold with  $\alpha(f, x) \equiv \alpha$  and let  $p \in \mathfrak{P}(\mathcal{X})$  be a probability step-function. Then we define the LFC of LLS in the non-isotropic, indefinite case as

$$\mathfrak{C}_{1,\mathbb{S}_{++}^d}^n(x) = \left[\frac{v(x)}{p(x)n}\right]^{\frac{d}{2\alpha+d}} \left|\Sigma_{1,\mathbb{S}_{++}^d}^n(x)\right|^{-1} = \left[\frac{v(x)}{p(x)}\right]^{\frac{d}{2\alpha+d}} D_n(x) + o_p\left[1\right].$$

Since we can show that  $D_n$  is a continuous function, almost everywhere, so is  $\mathfrak{C}^n_{1,\mathbb{S}^d_{++}}$ .

#### Appendix B.3. Non-isotropic Optimal Sampling

From here on, we assume the local properties to hold globally over the input space. That is, f is either definite or indefinite, almost everywhere. And if f is indefinite, then we assume  $\alpha(f, x) \equiv \alpha$  for some shared  $\alpha > 2$ .

When taking a look at a definite function f, the result of Theorem 10 generalizes straight-forward the non-isotropic case:

**Corollary B13.** Let  $v, q \in C^0(\mathcal{X}, \mathbb{R}_+)$  for a compact input space  $\mathcal{X}$ , where q is a test density such that  $\int_{\mathcal{X}} q(x)dx = 1$ . Additionally, assume that v and q are bounded away from zero. That is,  $v, q \geq \epsilon$  for some  $\epsilon > 0$ . Let k be a RBF-kernel with bandwidth parameter space  $\mathcal{S} = \mathbb{S}^d_{++}$ . Let  $f \in C^2(\mathcal{X})$  such

that f is definite, almost everywhere. Then the optimal training density for LLS is asymptotically given by

$$p_{O_{pt}}^{1,\mathbb{S}_{++}^d,n}(x) \propto \left[\mathfrak{C}_{1,\mathbb{S}_{++}^d}^n(x)q(x)\right]^{\frac{4+d}{8+d}} v(x)^{\frac{4}{8+d}}(1+o(1)).$$
(B.8)

*Proof.* Basically, the proof is analogous to the proof in Theorem 10, apart from the following adaptions: Instead of Corollary 6 we apply Corollary B4 for the asymptotic formulation of LOB. For the asymptotic variance, we apply (B.2) in Theorem B2 instead of (14) in Theorem 3. Instead of Definition 9 and (18), we apply Definition B8 and (B.7) for the LFC. With these, we can get to the point

$$MSE_1\left(x, \Sigma_{1, \mathbb{S}_{++}^d}^n(x) | \mathbf{X}_n\right) = \bar{C}_1\left[\frac{v(x)}{p(x)n}\right]^{\frac{4}{4+d}} \mathfrak{C}_{1, \mathbb{S}_{++}^d}^\infty(x) + o_p\left[n^{-\frac{4}{4+d}}\right],$$

with  $\bar{C}_1 = \frac{4+d}{4}R(k)C_1^{-d}$ , as in Theorem 10 from where we can proceed in complete analogy.

Here, extending the above results to the indefinite case poses a problem, since we cannot take the functional derivative with respect to step-function p. However, we suggest to use the straight-forward extension as a heuristic solution:

**Conjecture B14.** Let  $v, q \in C^0(\mathcal{X}, \mathbb{R}_+)$  for a compact input space  $\mathcal{X}$ , where q is a test density such that  $\int_{\mathcal{X}} q(x) dx = 1$ . Additionally, assume that v and q are bounded away from zero. That is,  $v, q \geq \epsilon$  for some  $\epsilon > 0$ . Let  $\alpha = L + \beta$  with  $L \in \mathbb{N}, L \geq 2$  and  $\beta \in (0, 1]$  with  $f \in C^{\alpha}(\mathcal{X})$  such that  $\alpha(f, x) \equiv \alpha$ , almost everywhere. Let  $k \in C^{\lfloor L/2 \rfloor}(\mathbb{R}_+, \mathbb{R}_+)$  be a RBF-kernel with bandwidth parameter space  $\mathcal{S} = \mathbb{S}_{++}^d$  for  $d \geq 2$ . Then, for almost everywhere indefinite f, the training density

$$p_{O_{pt}}^{1,\mathbb{S}_{++}^{d},n}(x) \propto \left[\mathfrak{C}_{1,\mathbb{S}_{++}^{d}}^{n}(x)q(x)\right]^{\frac{2\alpha+d}{4\alpha+d}}v(x)^{\frac{2\alpha}{4\alpha+d}}(1+o(1))$$
(B.9)

is asymptotically superior to random test sampling for LLS.

### Appendix C. Higher-order Bias Expansion

As already noted, the function f to infer will typically not be definite, almost everywhere. In the indefinite regime, the second-order bias-term can be eliminated systematically. Here, the straight-forward approach for extension of the analysis of LOB is to take higher-order bias-terms into consideration. Being mathematically more precise, we will now analyze the higher-order bias-decomposition.

**Proposition C1** (The asymptotic bias of *l*-th order). Assume the kernel k to be symmetric and let  $\alpha = L + \beta$  with  $L \in \mathbb{N}, L \geq 2$  and  $\beta \in (0, 1]$ . Furthermore let  $h_n = n^{-\frac{1}{2\alpha+d}}$ ,  $p \in C^{\alpha-2}(\mathcal{X})$  and  $f \in C^{\alpha}(\mathcal{X})$ . For a fixed  $x \in \mathcal{X}^{\circ}$  and  $\Sigma \in \mathbb{S}^d_{++}$  we can decompose the conditional bias of LLS as

$$\mathbb{B}_{1}\left[x, h_{n}\Sigma | \boldsymbol{X}_{n}\right] = \sum_{l=1}^{\lfloor L/2 \rfloor} bias_{1,2l}\left[x, h_{n}\Sigma\right] + O_{p}\left[h_{n}^{\alpha}\right].$$

The bias-terms of odd order vanish, whereas the bias-terms of even order are given by

$$bias_{1,2l} [x, \Sigma] = \sum_{j_1, \dots, j_{2l}=1}^{d} A^{l,x}_{j_1, \dots, j_{2l}} \sum_{i_1, \dots, i_{2l}=1}^{d} B^{l,x}_{i_1, \dots, i_{2l}} \prod_{r=1}^{2l} \Sigma_{i_r, j_r}, \qquad (C.1)$$

where the tensors  $A^{l,x}$  and  $B^{l,x}$  depend on derivatives (with a total order of 2l) in x of f of order 2 to 2l, and p up to order 2l - 2. In particular,  $bias_{1,2l}[x, \Sigma]$  is continuous in x.

*Proof.* Recall from (11) that

$$\mathbb{B}_1\left[x, \Sigma | \boldsymbol{X}_n\right] = f(x) - e_1^\top \left(X_1(x)^\top W_x^\Sigma X_1(x)\right)^{-1} X_1(x)^\top W_x^\Sigma f(\boldsymbol{X}_n).$$

Let

$$f(\boldsymbol{X}_n) = \sum_{l=0}^{L} T_l^{f,x}(\boldsymbol{X}_n) + O_p \left[ \|\boldsymbol{X}_n - x\|^{\alpha} \right]$$

be the Taylor expansion of the true training function values, where

$$T_l^{f,x}(\boldsymbol{X}_n) = \begin{bmatrix} T_l^{f,x}(x_1) & \dots & T_l^{f,x}(x_n) \end{bmatrix}^\top$$

are the Taylor expansion terms of l-th order of the respective training samples. That is,

$$T_l^{f,x}(x') = \frac{1}{l!} \sum_{i_1,\dots,i_l=1}^d [D_f^l(x)]_{i_1,\dots,i_l} \prod_{r=1}^l (x'-x)_{i_r}.$$

Defining  $N_x^{h_n \Sigma} = e_1^{\top} \left( \frac{1}{n} X_1(x)^{\top} W_x^{h_n \Sigma} X_1(x) \right)^{-1}$ , and noting that the first two

Taylor expansion terms can be written as  $X_1(x) \begin{bmatrix} f(x) & D_f(x) \end{bmatrix}^\top$ , we obtain

$$\begin{split} \mathbb{B}_{1}\left[x,h_{n}\Sigma|\boldsymbol{X}_{n}\right] \\ &= N_{x}^{h_{n}\Sigma}X_{1}(x)^{\top}W_{x}^{h_{n}\Sigma}\left[\frac{1}{n}\sum_{l=2}^{L}T_{l}^{f,x}(\boldsymbol{X}_{n}) + O_{p}\left[n^{-1}\|\boldsymbol{X}_{n}-x\|^{\alpha}\right]\right] \\ &= N_{x}^{h_{n}\Sigma}X_{1}(x)^{\top}W_{x}^{h_{n}\Sigma}\left[\frac{1}{n}\sum_{l=2}^{L}T_{l}^{f,x}(\boldsymbol{X}_{n})\right] + O_{p}\left[h_{n}^{\alpha}\right], \end{split}$$

Denoting  $\frac{1}{n}X_1(x)^{\top}W_x^{h_n\Sigma}X_1(x) = \begin{bmatrix} a & b^{\top} \\ b & C \end{bmatrix}$  with  $\begin{bmatrix} e & g^{\top} \\ g & H \end{bmatrix} = \begin{bmatrix} a & b^{\top} \\ b & C \end{bmatrix}^{-1}$ , we have  $N_x^{h_n\Sigma} = \begin{bmatrix} e & g^{\top} \end{bmatrix}$ . Note that in the following we can ignore the error from Monte Carlo integration, as its convergence error of  $n^{-\frac{1}{2}}$  is  $o_p [h_n^{\alpha}]$  for the optimal rate  $h_n \propto n^{-\frac{1}{2\alpha+d}}$ . Hence we can write

$$\begin{split} \begin{bmatrix} a & b^{\top} \\ b & C \end{bmatrix} &= \frac{1}{n} \sum_{i=1}^{n} k^{h_n \Sigma}(x_i, x) \begin{bmatrix} 1 & (x_i - x)^{\top} \\ x_i - x & (x_i - x)(x_i - x)^{\top} \end{bmatrix} \\ &= \int k(u) du \sum_{k=0}^{L-2} T_k^{p,x}(x + h_n \Sigma u) \begin{bmatrix} 1 & h_n u^{\top} \Sigma \\ h_n \Sigma u & h_n^2 \Sigma u u^{\top} \Sigma \end{bmatrix} \\ &+ O_p \left[ \begin{bmatrix} h_n^{\alpha-2} & h_n^{\alpha-1} \mathbb{1}_d^{\top} \\ h_n^{\alpha-1} \mathbb{1}_d & h_n^{\alpha} \mathbb{1}_d \mathbb{1}_d^{\top} \end{bmatrix} \right] \\ &= \begin{bmatrix} 1 & 0 \\ 0 & h_n \Sigma \end{bmatrix} \sum_{l=0}^{\lfloor (L-2)/2 \rfloor} \begin{bmatrix} P_a^{2l}(h_n \Sigma) & 0 \\ 0 & P_C^{2l}(h_n \Sigma) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & h_n \Sigma \end{bmatrix} \\ &+ \begin{bmatrix} 1 & 0 \\ 0 & h_n \Sigma \end{bmatrix} \sum_{l=0}^{\lfloor (L-3)/2 \rfloor} \begin{bmatrix} 0 & P_b^{2l+1}(h_n \Sigma)^{\top} \\ D_b^{2l+1}(h_n \Sigma) & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & h_n \Sigma \end{bmatrix} \\ &+ O_p \left[ \begin{bmatrix} h_n^{\alpha-2} & h_n^{\alpha-1} \mathbb{1}_d^{\top} \\ h_n^{\alpha-1} \mathbb{1}_d & h_n^{\alpha} \mathbb{1}_d \mathbb{1}_d^{\top} \end{bmatrix} \right], \end{split}$$

where all odd-order terms in  $\boldsymbol{u}$  vanish when integrating with respect to an RBF-kernel, and

$$P_{a}^{2l}(Z) := \int k(u) du T_{2l}^{p,x}(x + Zu)$$

$$P_{b}^{2l+1}(Z) := \int k(u) du T_{2l+1}^{p,x}(x + Zu) u$$

$$P_{C}^{2l}(Z) := \int k(u) du T_{2l}^{p,x}(x + Zu) uu^{\top}.$$

The denoted monomial order of these terms corresponds to the contained number of bandwidth matrices. The expansions of a, b and C depend on derivatives of p up to order L-2). As a function of  $h_n$ , when applying the chain-rule, there exists an expansion (in root h = 0)

$$C^{-1} = (h_n \Sigma)^{-1} \sum_{l=0}^{\lfloor (L-2)/2 \rfloor} P_{C^{-1}}^{2l} (h_n \Sigma) (h_n \Sigma)^{-1} + O_p \left[ h_n^{\alpha-4} \mathbbm{1}_d \mathbbm{1}_d^\top \right],$$

that can be constructed in terms of the expansion of C. Thus it will also depend on derivatives of p up to order (L-2). Aligning the adequate terms, we can therefore expand

$$b^{\top} C^{-1} b = \sum_{l=1}^{\lfloor (L-2)/2 \rfloor} P_{b^{\top} C^{-1} b}^{2l}(h_n \Sigma) + O_p \left[ h_n^{\alpha-2} \right].$$

Using the fact that  $e^{-1} = a - b^{\top} C^{-1} b$ , we also have

$$e^{-1} = P_a^0(h_n\Sigma) + \sum_{l=1}^{\lfloor (L-2)/2 \rfloor} \left[ P_a^{2l}(h_n\Sigma) - P_{b^\top C^{-1}b}^{2l}(h_n\Sigma) \right] + O_p \left[ h_n^{\alpha-2} \right],$$

where  $P_a^0(h_n\Sigma) = p(x)$ . Applying the chain-rule, the expansion of

$$e = \sum_{l=0}^{\lfloor (L-2)/2 \rfloor} P_e^{2l}(h_n \Sigma) + O_p \left[ h_n^{\alpha-2} \right]$$

exists and also depend on derivatives of p up to order (L-2). Note that  $P^0_e(h_n\Sigma)=p(x)^{-1}.$ 

Using the fact that  $g^{\top} = -eb^{\top}C^{-1}$ , with adequate alignment of the terms of their expansions, it is

$$\boldsymbol{g}^{\top} = \sum_{l=0}^{\lfloor (L-3)/2 \rfloor} \boldsymbol{P}_{\boldsymbol{g}}^{2l+1} (\boldsymbol{h}_{n}\boldsymbol{\Sigma})^{\top} (\boldsymbol{h}_{n}\boldsymbol{\Sigma})^{-1} + \boldsymbol{O}_{p} \left[ \boldsymbol{h}_{n}^{\alpha-3} \mathbb{1}_{d}^{\top} \right]$$

which does depend on derivatives of p up to order (L-2). Note that, if  $L \geq 3$ , then  $P_g^1(h_n \Sigma)^{\top} = -D_p^1(x)p(x)^{-2}h_n\Sigma$ . Therefore

$$\begin{split} N_x^{h_n\Sigma} = \begin{bmatrix} \lfloor (L-2)/2 \rfloor \\ \sum_{l=0}^{\lfloor l} P_e^{2l}(h_n\Sigma) & \sum_{l=0}^{\lfloor L-3)/2 \rfloor} P_g^{2l+1}(h_n\Sigma)^\top \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & h_n\Sigma \end{bmatrix}^{-1} \\ + O_p \left[ \begin{bmatrix} h_n^{\alpha-2} & h_n^{\alpha-3} \mathbb{1}_d^\top \end{bmatrix} \right]. \end{split}$$

Now we can also expand

$$\begin{split} \frac{1}{n} X_1(x)^\top W_x^{h_n \Sigma} T_l^{f,x}(\boldsymbol{X}_n) &= \frac{1}{n} \sum_{i=1}^n k^{h_n \Sigma}(x, x_i) T_l^{f,x}(x_i) \begin{bmatrix} 1\\ x_i - x \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0\\ 0 & h_n \Sigma \end{bmatrix} \int k(u) du T_l^{f,x}(x + h_n \Sigma u) \cdot \sum_{r=0}^{L-l} T_r^{p,x}(x + h_n \Sigma u) \begin{bmatrix} 1\\ u \end{bmatrix} \\ &+ O_p \left[ \begin{bmatrix} h_n^\alpha & h_n^{\alpha+1} \mathbb{1}_d^\top \end{bmatrix}^\top \right]. \end{split}$$

Note that here also all odd-order terms in u vanish for RBF-kernels. Aggregating the polynomial terms of  $\frac{1}{n}X_1(x)^{\top}W_x^{h_n\Sigma}\left[\sum_{l=2}^L T_l^{f,x}(\boldsymbol{X}_n)\right]$  of total order 2l, we obtain

$$b_{2l}(x,h_n\Sigma) = \begin{bmatrix} 1 & 0\\ 0 & h_n\Sigma \end{bmatrix} \int k(u)du \begin{bmatrix} \sum_{r=2}^{2l} T_r^{f,x}(x+h_n\Sigma u) T_{2l-r}^{p,x}(x+h_n\Sigma u)\\ \sum_{r=2}^{2l-1} T_r^{f,x}(x+h_n\Sigma u) T_{2l-1-r}^{p,x}(x+h_n\Sigma u)u \end{bmatrix}.$$

Subsequently, when multiplying  $\frac{1}{n}X_1(x)^{\top}W_x^{h_n\Sigma}\left[\sum_{l=2}^{L}T_l^{f,x}(\boldsymbol{X}_n)\right]$  and  $N_x^{h_n\Sigma}$ , any combination of an explicit term with an  $O_p$ -term is in  $O_p[h_n^{\alpha}]$ . Particularly, multiplying  $O_p\left[\begin{bmatrix}h_n^{\alpha-2} & h_n^{\alpha-3}\mathbb{1}_d^{\top}\end{bmatrix}\right]$  with any  $b_{2l}$ -term is  $O_p[h_n^{\alpha}]$ , because  $b_2(x,h_n\Sigma) = O_p\left[\begin{bmatrix}h_n^2 & 0\end{bmatrix}^{\top}\right]$  and  $b_4(x,h_n\Sigma) = O_p\left[h_n^4\mathbb{1}_{d+1}\right]$ . Finally, we can decompose the conditional bias as

inary, we can decompose the conditional bias as

$$\mathbb{B}_{1}\left[x, h_{n} \Sigma | \boldsymbol{X}_{n}\right] = \sum_{l=1}^{\lfloor L/2 \rfloor} \operatorname{bias}_{1,2l}\left[x, h_{n} \Sigma\right] + O_{p}\left[h_{n}^{\alpha}\right],$$

where the bias of order 2l is given by

$$bias_{1,2l}[x, Z] = \sum_{m=1}^{l} \left[ P_e^{2(l-m)}(Z) \quad P_g^{2(l-m)+1}(Z)^\top \right]$$
$$\begin{bmatrix} \sum_{r=2}^{2m} \int T_r^{f,x}(x+Zu) T_{2m-r}^{p,x}(x+Zu)k(u)du\\ \sum_{r=2}^{2m-1} \int T_r^{f,x}(x+Zu) T_{2m-1-r}^{p,x}(x+Zu)uk(u)du \end{bmatrix}.$$

Via construction,  $\operatorname{bias}_{1,2l}[x, \Sigma]$  depends on derivatives of f of second or higher-order, and p (with a total order of 2l). The maximal orders are

therefore (2l-2) for p and 2l for f. Denote by  $A^{l,x}$  and  $B^{l,x}$  the adequate coefficient-tensors. Then we can write

$$\operatorname{bias}_{1,2l}[x,h_n\Sigma] = h_n^{2l} \sum_{j_1,\dots,j_{2l}=1}^d A_{j_1,\dots,j_{2l}}^{l,x} \sum_{i_1,\dots,i_{2l}=1}^d B_{i_1,\dots,i_{2l}}^{l,x} \prod_{r=1}^{2l} \Sigma_{i_r,j_r}.$$

Note that all odd-order bias-terms vanish by symmetry of the kernel k. The higher-order bias-decomposition enormously simplifies under the assumption of uniformly distributed inputs:

**Corollary C2.** May the assumptions of Proposition C1 hold. If additionally  $p \sim \mathcal{U}(\mathcal{X})$  is uniformly distributed, the asymptotic even-order bias-terms simplify to

$$bias_{1,2l} [x, \Sigma] = \sum_{i_1, \dots, i_{2l}=1}^d \frac{\mu(i_1, \dots, i_{2l})}{(2l)!} \sum_{j_1, \dots, j_{2l}=1}^d [D_f^{2l}(x)]_{j_1, \dots, j_{2l}} \prod_{r=1}^{2l} \Sigma_{i_r j_r},$$

where  $\mu(i_1, \ldots, i_{2l}) = \prod_{p=1}^d \mu_{c_p(i_1, \ldots, i_{2l})}$  for  $\mu_c = \int u^c k(u) du$  the moments of the RBF-kernel k with  $\mu_0 = 1$  (such that k is a probability density on  $\mathbb{R}^d$ ) and  $c_p(i_1, \ldots, i_{2l}) = |\{r \mid i_r = p\}|.$ 

*Proof.* In the case of  $p \sim \mathcal{U}(\mathcal{X})$ , the only non-vanishing term in  $\operatorname{bias}_{1,2l}[x, \Sigma]$  from (C.1) is

$$\underbrace{\underline{P}_{e}^{0}(\Sigma)}_{p(x)^{-1}} \int T_{2l}^{f,x}(x+\Sigma u) \underbrace{\underline{T}_{0}^{p,x}(x+\Sigma u)}_{p(x)} k(u) du = \int T_{2l}^{f,x}(x+\Sigma u)k(u) du$$
$$= \frac{1}{(2l)!} \sum_{j_{1},\dots,j_{2l}=1}^{d} [D_{f}^{2l}(x)]_{j_{1},\dots,j_{2l}} \int k(u) \prod_{r=1}^{2l} (\Sigma u)_{j_{r}} du$$
$$= \sum_{i_{1},\dots,i_{2l}=1}^{d} \frac{\mu(i_{1},\dots,i_{2l})}{(2l)!} \sum_{j_{1},\dots,j_{2l}=1}^{d} [D_{f}^{2l}(x)]_{j_{1},\dots,j_{2l}} \prod_{r=1}^{2l} \Sigma_{i_{r}j_{r}}.$$

**Remark C3.** The second-order bias of LLS does not depend on the training density p in general. Therefore it holds for an arbitrary, smooth enough p

that

$$\begin{split} bias_{1,2} \left[ x, \Sigma \right] \\ &= \sum_{i_1, i_2 = 1}^d \frac{\mu(i_1, i_2)}{2} \sum_{j_1, j_2 = 1}^d [D_f^2(x)]_{j_1, j_2} \prod_{r=1}^2 \Sigma_{i_r j_r} = \sum_{i=1}^d \frac{\mu_2}{2} \sum_{j_1, j_2 = 1}^d [D_f^2(x)]_{j_1, j_2} \prod_{r=1}^2 \Sigma_{i_j, j_j} \\ &= \frac{\mu_2}{2} \sum_{i=1}^d \left[ \Sigma D_f^2(x) \Sigma \right]_{i,i} = \frac{\mu_2}{2} \operatorname{trace}(\Sigma D_f^2(x) \Sigma) = \frac{\mu_2}{2} \operatorname{trace}(D_f^2(x) \Sigma^2). \end{split}$$

While this simplifies form of the bias is still quite tedious, all appearing terms are now at least given in explicit form. This enables the construction of a toy-example, as given in the next section.

### Appendix D. A minimal indefinite Toy-Example

As a preconsideration, let  $\mathcal{T}_{l}^{x} = \left\{ \Sigma \in \mathbb{S}_{++}^{d} \mid \operatorname{bias}_{1,2l}[x, \Sigma] = 0 \right\}$  be the vanishing sets of the respective, even-order bias-terms. We observe that  $\mathcal{T}_1^x = \left\{ \Sigma \in \mathbb{S}^d_{++} \ \Big| \ \textit{trace}(D^2_f(x)\Sigma^2) = 0 \right\} \text{ is a sub-manifold of } \mathbb{S}^d_{++} \text{ of at most}$  $(\dim(\mathbb{S}^{d}_{++})-1)$  dimensions for  $D^{2}_{f}(x) \neq 0$ . Letting  $\mathcal{S} \subseteq \mathbb{S}^{d}_{++}$  be our bandwidth candidate space, we thus assume that the candidate subspace  $\mathcal{S} \cap \bigcap_{l=0}^{L} T_{l}^{x}$ which simultaneously eliminates bias-terms up to order 2L will shrink and finally vanish as we increase L. Under mild assumptions on f and p we can assume that this subspace decreases in dimension by at least 1 with each consecutive conditioning on the elimination of the next higher-order bias-term. We end up with a bias-term of maximal order 2D that cannot be eliminated anymore, where  $D = \dim(S) \leq \frac{d(d+1)}{2}$ . This suggests that we could obtain minimax-optimal convergence for a generic  $f \in \tilde{\mathcal{C}}^{2D}(\mathcal{X})$ , when applying LLS with  $\mathcal{S}$ : While being infeasible from the practical point-of-view, we could construct LOB by first finding the subspace of  $\mathcal{S}$  that simultaneously eliminates as many leading-order bias terms as possible, followed by optimizing the trade-off between the first non-vanishing bias-term and the variance over this bandwidth candidate subspace.

The reasoning above however turns out to be naively pessimistic, since LOB does not necessarily lie in the specified terminal subspace. The true behavior of LOB is surprisingly different, and we will now construct a toyexample to reveal the principle.

Let  $\mathcal{X} = [0, 1]^2$  with uniformly distributed inputs  $p \sim \mathcal{U}(\mathcal{X})$  and observations  $p(y|x) = \mathcal{N}(y; f(x), v(x))$ , with

$$f(x) = \exp\{ax_1\} + \log(0.1 + bx_2)$$
 and  $v(x) = 10^{-4}$ 



Figure D.1: The bias canceling experiment: An example dataset (left). The two components (middle and right) of the naive anisotropic bandwidth construction up to the global scaling in n, as a means to estimate anisotropic LOB.

where we have set a = 2 and b = 3. An example dataset can be seen to the left in Fig. D.1. Furthermore let  $k(z) = \exp\{-0.5||z||^2\}$  be the Gaussian kernel and  $S = \{ diag(\sigma_1, \sigma_2) | \sigma_1, \sigma_2 > 0 \}$  the set of anisotropic bandwidths. The Hessian of f is given by

$$D_f^2(x)_{i_1,i_2} = \begin{cases} D_f^2(x)_1 := a^2 \exp\{ax_1\} &, i_1 = i_2 = 1, \\ D_f^2(x)_2 := -b^2(0.1 + bx_2)^{-2} &, i_1 = i_2 = 2, \\ 0 &, \text{ else,} \end{cases}$$

whereas the fourth-order partial derivatives are given by

$$D_f^4(x)_{i_1,\dots,i_4} = \begin{cases} D_f^4(x)_1 := a^4 \exp\{ax_1\} &, i_1 = \dots = i_4 = 1, \\ D_f^4(x)_2 := -6b^4(0.1 + bx_2)^{-4} &, i_1 = \dots = i_4 = 2, \\ 0 &, \text{ else.} \end{cases}$$

Recall from (B.1) that the second-order bias is given by  $\operatorname{bias}_{1,2}[x, \Sigma] = \frac{1}{2}\mu_2 \operatorname{trace}(D_f^2(x)\Sigma^2)$ . In the isotropic case,  $\operatorname{bias}_{1,2}[x, \sigma \mathcal{I}_d]$  will vanish almost nowhere. Letting  $\Sigma_2(x) \equiv \mathcal{I}_d$ , and when optimizing

$$MSE_1(x, \sigma \Sigma_2(x) | \boldsymbol{X}_n) = bias_{1,2} [x, \sigma \Sigma_2(x)]^2 + var_1 [x, \sigma \Sigma_2(x) | \boldsymbol{X}_n] + o_p \left[ \sigma^4 + n^{-1} \sigma^{-d} \right]$$

with respect to  $\sigma,$  the optimum is obtained for  $\sigma^*=h_{2,n}\sigma_2^*(x),$  where  $h_{2,n}=n^{-\frac{1}{4+d}}$  and

$$\sigma_2^*(x) = \left[\frac{R(k)v(x)d}{4p(x) |\Sigma_2(x)| \operatorname{bias}_{1,2} [x, \Sigma_2(x)]^2}\right]^{\frac{1}{4+d}}$$

Defining

$$\Sigma_2^n(x) = h_{2,n} \sigma_2^*(x) \Sigma_2(x),$$

the associated performance law is then given by

MSE<sub>1</sub> 
$$(x, \Sigma_2^n(x) | \mathbf{X}_n) = O_p \left[ h_{2,n}^4 \right] = O_p \left[ n^{-\frac{4}{4+d}} \right].$$

Note that the choice of the spatial component  $\sigma_2^*(x)$  only influences the MSE by a constant factor, whereas the global decay rate  $h_{2,n}$  affects the decay law of the MSE.

Further note that, if the leading bias-term vanishes for some  $x \in \mathcal{X}$ , the asymptotic analysis suggests  $\sigma_2^*(x_i) \to \infty$  as  $x_i \to x$ . In contrast, when dealing with finite data, the remaining higher-order bias – which is not treated in this case – would prevent the real LOB from exploding. Such roots of the leading bias-term – even if only occurring on a set of measure zero – will therefore negatively impact the MSE on a substantial share of the input space. Since our example suffers from such roots, i.e., for  $x_1 = a^{-1} \log(b^2(0.1 + bx_2)^{-2}a^{-2})$ , and since we focus on the decay law as opposed to the optimal constant of the MSE, we suggest to trade off the general scaling of the bias in  $\Sigma$  and  $|\Sigma|$  in a label-agnostic way, being more robust. Therefore we will replace bias<sub>1,2</sub>  $[x, \Sigma_2(x)]$  with  $\|\Sigma_2(x)\|^2$  in  $\sigma_2^*$ .

In the anisotropic case, when following the naive approach, we would first estimate  $\mathcal{T}_1^x = \{\Sigma \in \mathcal{S} \mid \text{bias}_{1,2} [x, \Sigma] = 0\} = \{\Sigma \in \mathcal{S} \mid \text{trace}(D_f^2(x)\Sigma^2) = 0\},\$ which is given in particular by  $\mathcal{T}_1^x = \{\sigma \Sigma_4(x) \mid \sigma > 0\},\$ where

$$\Sigma_4(x) = diag(1, s_4(x))$$
 with  $s_4(x) = \sqrt{-D_f^2(x)_1/D_f^2(x)_2}$ .

Over  $\mathcal{T}_1^x$ , we then optimize

$$MSE_1(x, \sigma \Sigma_4(x) | \boldsymbol{X}_n) = bias_{1,4} [x, \sigma \Sigma_4(x)]^2 + var_1 [x, \sigma \Sigma_4(x) | \boldsymbol{X}_n] + o_p \left[\sigma^8 + n^{-1} \sigma^{-d}\right]$$

with respect to  $\sigma$ , where  $\operatorname{bias}_{1,4}[x, \sigma \Sigma_4(x)] = \frac{\mu_4}{24} \sigma^4 (D_f^4(x)_1 + s_4(x)^4 D_f^4(x)_2) = O_p\left[\sigma^4 \|\Sigma_4(x)\|^4\right]$ . Hence, the optimum is obtained for  $\sigma^* = h_{4,n}\sigma_4^*(x)$ , where  $h_{4,n} = n^{-\frac{1}{8+d}}$  and

$$\sigma_4^*(x) = \left[\frac{R(k)v(x)d}{8p(x) |\Sigma_4(x)| \operatorname{bias}_{1,4} [x, \Sigma_4(x)]^2}\right]^{\frac{1}{8+d}}.$$



Figure D.2: The bias canceling experiment: The ratio of the two components of the improved and the naive anisotropic bandwidth construction, evaluated at  $h_n = 0.1$ .

Therefore the optimal bandwidth in x with this construction is asymptotically given by

$$\Sigma_4^n(x) = h_{4,n}\sigma_4^*(x)\Sigma_4(x),$$

with the associated improved performance law

$$\mathrm{MSE}_{1}\left(x,\Sigma_{4}^{n}(x)|\boldsymbol{X}_{n}\right) = O_{p}\left[h_{4,n}^{8}\right] = O_{p}\left[n^{-\frac{8}{8+d}}\right].$$

For the same stability reasons as in the isotropic case, and since we focus on the decay-law, we replace  $\operatorname{bias}_{1,4}[x, \Sigma_4(x)]$  with  $\|\Sigma_4(x)\|^4$  in  $\sigma_4^*$ . We have plotted this bandwidth construction in Fig. D.1 (middle and right).

While the construction above seems intuitive through its straight-forward calculation, it is not optimal. We will now show, that the vanishing second-order bias can be exploited to delete the fourth-order bias. The sequence of bandwidths  $(\Sigma_6^n(x))_{n\in\mathbb{N}}$  that features this property will then follow the performance law

$$\mathrm{MSE}_1\left(x, \Sigma_6^n(x) | \boldsymbol{X}_n\right) = O_p\left[n^{-\frac{12}{12+d}}\right].$$

An empirical comparison of LOB and MSE decay laws obtained by the three constructions can be found in Fig. D.3. Note that while this is still not the optimal law, it confirms the sub-optimality of the naive construction and demonstrates the true principle that LOB follows in non-isotropic scenarios.

The asymptotic forms of bias and variance were derived for a fixed  $\Sigma$ , where only the rate  $h_n$  changes with n. For example, for a fixed  $\Sigma$  consider the fourth-order expansion

$$\mathbb{B}_{1}\left[x, h_{n}\Sigma | \boldsymbol{X}_{n}\right] = \operatorname{bias}_{1,2}\left[x, h_{n}\Sigma\right] + \operatorname{bias}_{1,4}\left[x, h_{n}\Sigma\right] + o_{p}\left[h_{n}^{4}\right]$$



Figure D.3: The bias canceling experiment: Empirical results and theoretically given, asymptotic decay laws of the global scaling (left) and the achieved MISE (right) in the isotropic, naive anisotropic and improved anisotropic bandwidth case. The experimental results are averaged over 10 repetitions. The MISE is measured on the interior  $[0.1, 0.9]^2$  of the input space.

When we seek for a sequence  $\Sigma_x^n$  that eliminates the fourth-order biasterm by the second-order bias-term, we cannot simply solve the asymptotic equation

$$h_n^4 \text{bias}_{1,4} [x, \Sigma_x^n] = -h_n^2 \text{bias}_{1,2} [x, \Sigma_x^n],$$

in order to obtain  $\mathbb{B}_1[x, h_n \Sigma_x^n | \mathbf{X}_n] = o_p[h_n^4]$ . This is because the asymptotic form holds not true in first place for a changing  $\Sigma_x^n$  in n. We address this issue as follows. For an arbitrary function  $F \in \mathcal{C}^0(\mathcal{X})$  consider its Monte Carlo integration

$$\frac{1}{n} \sum_{i=1}^{n} k^{\Sigma}(x_i - x) F(x_i) = \int k(u) p(x + \Sigma u) F(x + \Sigma u) du + O(n^{-\frac{1}{2}}).$$

The proof of Proposition C1 is based on Taylor-expansions of several such terms: Recall that

$$\mathbb{B}_1\left[x, h_n \Sigma | \boldsymbol{X}_n\right] = N_x^{h_n \Sigma} X_1(x)^\top W_x^{h_n \Sigma} \left[\frac{1}{n} \sum_{l=2}^L T_l^{f,x}(\boldsymbol{X}_n)\right] + o_p\left[h_n^L\right],$$

where it was

$$N_x^{h_n\Sigma} = e_1^{\top} \left( \frac{1}{n} \sum_{i=1}^n k^{h_n\Sigma}(x_i, x) \begin{bmatrix} 1 & (x_i - x)^{\top} \\ x_i - x & (x_i - x)(x_i - x)^{\top} \end{bmatrix} \right)^{-1}$$

and

$$X_1(x)^\top W_x^{h_n \Sigma} \left[ \frac{1}{n} T_l^{f,x}(\boldsymbol{X}_n) \right] = \frac{1}{n} \sum_{i=1}^n k^{h_n \Sigma}(x_i, x) \begin{bmatrix} 1\\ x_i - x \end{bmatrix} T_l^{f,x}(x_i).$$

Now, the first derivative of the Gaussian kernel with respect to the bandwidth is given by

$$\frac{\partial k^{\Sigma}(z)}{\partial \Sigma} = -k^{\Sigma}(z)(\mathcal{I}_d - \Sigma^{-1} z z^{\top} \Sigma^{-1}) \Sigma^{-1}.$$

For  $\Sigma = diag(\sigma_1, \ldots, \sigma_d)$ , the second derivative of the Gaussian kernel is given by

$$\frac{\partial^2 k^{\Sigma}(z)}{\partial \sigma_i \partial \sigma_j} = k^{\Sigma}(z) \left[ (1 - \frac{z_i^2}{\sigma_i^2})(1 - \frac{z_j^2}{\sigma_j^2}) + \delta_{ij}(1 - 3\frac{z_i^2}{\sigma_i^2}) \right].$$

Now, let  $x \in \mathcal{X}$  and  $\Sigma_x = diag(\sigma_1, \sigma_2) \in \mathcal{S}$  be fixed. For a sequence  $\Sigma_x^n = diag(\sigma_1^n, \sigma_2^n)$  we define  $\varepsilon_n = \|\Sigma_x^{-1}(\Sigma_x^n - \Sigma_x)\|$ . If  $h_n, \varepsilon_n = o_p[1]$ , we can expand

$$\begin{split} &\frac{1}{n} \sum_{i=1}^{n} k^{h_n \Sigma_x^n} (x_i - x) F(x_i) \\ &= \frac{1}{n} \sum_{i=1}^{n} F(x_i) k^{h_n \Sigma_x} (x_i - x) \left[ 1 - \sum_{j=1}^{d} [1 - \frac{z_j^2}{\sigma_j^2}] [\frac{\sigma_j^n}{\sigma_j} - 1] \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ [1 - \frac{z_j^2}{\sigma_j^2}] [1 - \frac{z_k^2}{\sigma_k^2}] + \delta_{j,k} [1 - 3\frac{z_j^2}{\sigma_j^2}] \right] [\frac{\sigma_j^n}{\sigma_j} - 1] [\frac{\sigma_k^n}{\sigma_k} - 1] + o_p \left[ \varepsilon_n^2 \right] \\ &= \int du k(u) p(x + h_n \Sigma_x u) F(x + h_n \Sigma_x u) \left[ 1 - \sum_{j=1}^{d} [1 - u_j^2] [\frac{\sigma_j^n}{\sigma_j} - 1] \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ [1 - u_j^2] [1 - u_k^2] + \delta_{j,k} [1 - 3u_j^2] \right] [\frac{\sigma_j^n}{\sigma_j} - 1] [\frac{\sigma_k^n}{\sigma_k} - 1] + o_p \left[ \varepsilon_n^2 \right] \\ &= \int du k(u) p(x + h_n \Sigma_x u) F(x + h_n \Sigma_x u) \left[ 1 - \sum_{j=1}^{d} [1 - u_j^2] [\frac{\sigma_j^n}{\sigma_j} - 1] \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ [1 - u_j^2] [1 - u_k^2] + \delta_{j,k} [1 - 3u_j^2] \right] [\frac{\sigma_j^n}{\sigma_j} - 1] [\frac{\sigma_k^n}{\sigma_k} - 1] + o_p \left[ \varepsilon_n^2 \right] \\ &= \int du k(u) p(x + h_n \Sigma_x u) F(x + h_n \Sigma_x u) \left[ 1 - \sum_{j=1}^{d} [1 - u_j^2] [\frac{\sigma_j^n}{\sigma_j} - 1] \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ [1 - u_j^2] [1 - u_k^2] + \delta_{j,k} [1 - 3u_j^2] \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_k} - 1 \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ [1 - u_j^2] [1 - u_k^2] + \delta_{j,k} [1 - 3u_j^2] \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_k} - 1 \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{1}{2} \sum_{j,k=1}^{d} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{\sigma_j^n}{\sigma_j} \left[ \frac{\sigma_j^n}{\sigma_j} - 1 \right] \\ &+ \frac{\sigma_j^$$

We first consider  $F(z) := T_2^{f,x}(z) = \frac{1}{2}(z-x)^{\top} D_f^2(x)(z-x)$  in order to deal with the second-order bias. Here, we can choose the fixed bandwidth  $\Sigma_x = \sigma \Sigma_4(x) \in \mathcal{T}_1^x$  such that  $\operatorname{bias}_{1,2}[x, \Sigma_x] = 0$ , which removes the second-order error. Additionally, we set up the candidate solution  $\Sigma_x^n = \sigma \operatorname{diag}(1, s_6^n(x))$ . We then observe that  $\frac{\sigma_1^n}{\sigma_1} - 1 = 0$  and  $\frac{\sigma_2^n}{\sigma_2} - 1 = \frac{s_6^n(x)}{s_4(x)} - 1 = \varepsilon_n$ . With  $p \equiv 1$  it

$$\begin{split} &\frac{1}{n} \sum_{i=1}^{n} k^{h_n \Sigma_n^n} (x_i - x) T_2^{f,x} (x_i) + o_p \left[ h_n^2 \varepsilon_n^2 \right] \\ &= \int du k(u) T_2^{f,x} (x + h_n \Sigma_x u) \left[ 1 - \varepsilon_n [1 - u_2^2] + \frac{1}{2} \varepsilon_n^2 ([1 - u_2^2]^2 + [1 - 3u_2^2]) \right] \\ &= \underbrace{\text{bias}_{1,2} \left[ x, h_n \Sigma_x \right]}_{=0} (1 - \varepsilon_n + \varepsilon_n^2) + \frac{1}{2} h_n^2 \sigma^2 \left[ \varepsilon_n \left[ D_f^2(x)_1 \mu_2^2 + \underbrace{s_4(x)^2 D_f^2(x)_2}_{-D_f^2(x)_1} \mu_4 + \frac{1}{2} \varepsilon_n^2 \left[ D_f^2(x)_1 (\mu_2 \mu_4 - 5\mu_2^2) + s_4(x)^2 D_f^2(x)_2 (\mu_6 - 5\mu_4) \right] \right] \\ &= \frac{1}{2} h_n^2 \sigma^2 \left[ \varepsilon_n D_f^2(x)_1 \left[ \mu_2^2 - \mu_4 \right] + \frac{1}{2} \varepsilon_n^2 D_f^2(x)_1 \left[ \mu_2 \mu_4 - 5\mu_2^2 - \mu_6 + 5\mu_4 \right] \right]. \end{split}$$

Analogously, when dealing with the fourth-order bias, we set

$$F(z) := T_4^{f,x}(z) = \frac{1}{24} \left[ (z_1 - x_1)^4 D_f^4(x)_1 + (z_2 - x_2)^4 D_f^4(x)_2 \right],$$

giving

$$\begin{split} \frac{1}{n} \sum_{i=1}^{n} k^{h_n \Sigma_x^n}(x, x_i) T_4^{f, x}(x_i) + O_p \left[ h_n^4 \varepsilon_n^2 \right] \\ &= h_n^4 \sigma^4 \text{bias}_{1,4} \left[ x, \Sigma_4(x) \right] \\ &\quad - \frac{h_n^4 \sigma^4}{24} \int du k(u) [u_1^4 D_f^4(x)_1 + u_2^4 s_4(x)^4 D_f^4(x)_2] \varepsilon_n [1 - u_2^2] \\ &= h_n^4 \sigma^4 \text{bias}_{1,4} \left[ x, \Sigma_4(x) \right] \\ &\quad + \frac{h_n^4 \sigma^4 \varepsilon_n}{24} \left[ D_f^4(x)_1 [\mu_2 \mu_4 - \mu_4] + s_4(x)^4 D_f^4(x)_2 [\mu_6 - \mu_4] \right]. \end{split}$$

Finally, we can write  $N_x^{h_n \Sigma} = \begin{bmatrix} 1 + o_p \begin{bmatrix} \varepsilon_n^2 \end{bmatrix} & 0 \end{bmatrix}$ . Therefore we can expand

$$\begin{split} \mathbb{B}_1\left(x,h_n\Sigma_x^n|\boldsymbol{X}_n\right) = &\frac{1}{2}h_n^2\sigma^2\varepsilon_nD_f^2(x)_1\left[\mu_2^2-\mu_4\right] \\ &+h_n^4\sigma^4\mathrm{bias}_{1,4}\left[x,\Sigma_4(x)\right] + O_p\left[h_n^2\varepsilon_n^2+h_n^4\varepsilon_n+h_n^6\right]. \end{split}$$

We can solve  $\mathbb{B}_1(x, h_n \Sigma_x^n | \mathbf{X}_n) = O_p \left[ h_n^2 \varepsilon_n^2 + h_n^4 \varepsilon_n + h_n^6 \right]$  for  $s_6^n(x)$ , recalling that  $\varepsilon_n = s_6^n(x) / s_4(x) - 1$ , which gives

$$s_6^n(x) = s_4(x) \left( 1 - \frac{2h_n^2 \sigma^2 \text{bias}_{1,4} \left[ x, \Sigma_4(x) \right]}{D_f^2(x)_1 \left[ \mu_2^2 - \mu_4 \right]} \right).$$

is

With this, it is  $\varepsilon_n = O_p \left[h_n^2\right]$  such that  $\mathbb{B}_1(x, h_n \Sigma_x^n | \mathbf{X}_n) = O_p \left[h_n^6\right]$ . Applying  $\Sigma_6^n(x) = \sigma diag(1, s_6^n(x))$ , we finally aggregate all sixth-order

Applying  $\Sigma_6^n(x) = \sigma diag(1, s_6^n(x))$ , we finally aggregate all sixth-order bias-terms that arise as  $\mathbb{B}(x, \Sigma_6^n(x) | \mathbf{X}_n) = \sigma^6 b_6(x, \Sigma_4(x)) + o_p[\sigma^6]$ , where

$$\begin{split} b_6(x, \Sigma_4(x)) &= \operatorname{bias}_{1,6} \left[ x, \Sigma_4(x) \right] \\ &+ \frac{1}{4} \left( \frac{2 \operatorname{bias}_{1,4} \left[ x, \Sigma_4(x) \right]}{D_f^2(x)_1 \left[ \mu_2^2 - \mu_4 \right]} \right)^2 D_f^2(x)_1 \left[ \mu_2 \mu_4 - 5\mu_2^2 - \mu_6 + 5\mu_4 \right] \\ &+ \frac{1}{24} \left( \frac{2 \operatorname{bias}_{1,4} \left[ x, \Sigma_4(x) \right]}{D_f^2(x)_1 \left[ \mu_2^2 - \mu_4 \right]} \right) \left[ D_f^4(x)_1(\mu_2 \mu_4 - \mu_4) + s_4(x)^4 D_f^4(x)_2(\mu_6 - \mu_4) \right], \end{split}$$

and  $\operatorname{bias}_{1,6}[x, \Sigma_4(x)] = \frac{\mu_6}{720} \left[ D_f^6(x)_1 + D_f^6(x)_2 s_4(x)^6 \right]$ . Accordingly, we write

$$MSE_{1}(x, \Sigma_{6}^{n}(x) | \boldsymbol{X}_{n}) = \sigma^{12} b_{6}(x, \Sigma_{4}(x))^{2} + \operatorname{var}_{1}[x, \sigma \Sigma_{4}(x) | \boldsymbol{X}_{n}] + o_{p} \left[ \sigma^{12} + n^{-1} \sigma^{-d} \right].$$

Here, the optimum is obtained for  $\sigma^* = h_{6,n} \sigma_6^*(x)$ , where  $h_{6,n} = n^{-\frac{1}{12+d}}$  and

$$\sigma_6^*(x) = \left[\frac{R(k)v(x)d}{12p(x)|\Sigma_4(x)|b_6(x,\Sigma_4(x))^2}\right]^{\frac{1}{12+d}}.$$

Thus, for  $\Sigma_6^n(x) = h_{6,n}\sigma_6^*(x) diag(1, s_6^n(x))$ , it is

$$MSE_1(x, \Sigma_6^n(x) | \boldsymbol{X}_n) = O_p\left[h_{6,n}^{12}\right] = O_p\left[n^{-\frac{12}{12+d}}\right]$$

Like in the previous cases we replace  $b_6(x, \Sigma_4(x))$  with  $\|\Sigma_4(x)\|^6$  in  $\sigma_6^*$ . We have plotted this bandwidth construction relative to the native, anisotropic construction in Fig. D.2.

So the trick is not to eliminate each respective higher-order bias-term on its own, but to abuse the slow convergence of the second-order bias-term together with a systematic deviation from its root in order to generate an anti-bias that cancels the effect of higher-order bias-terms. Note that this phenomenon works only in the direction of canceling higher-order bias from strictly vanishing lower-order bias and not vice versa. Following the concept of the toy-example, we are now in the position to analyze locally optimal non-isotropic bandwidths of LLS in the indefinite regime.

#### Appendix E. Non-isotropic LOB of LLS for indefinite functions

In the following, we focus on the interior of the input space, denoted by  $\mathcal{X}^{\circ}$ , and assume the kernel function k to be of bounded support. In particular,
let s > 0 such that  $k(t) \equiv 0, \forall t > s$ . When analyzing the asymptotics of LPS, we generally make the following consistency requirement on the applied bandwidth matrix as the sample size grows (see Ruppert and Wand (1994)):

**Definition E1.** A bandwidth sequence  $(\Sigma^n)_{n \in \mathbb{N}}$  is consistent, if

 $|\Sigma^n|^{-1} n^{-1} \to 0, \qquad \|\Sigma^n\| \to 0 \quad and \qquad \|\Sigma^n\| \cdot \|[\Sigma^n]^{-1}\| \le \mathcal{M}$ 

for some global constant  $1 \leq \mathcal{M} < \infty$ .

These requirements are necessary – though not sufficient – to make the LLS predictor weakly universally consistent in first place: The first two requirements are known from the isotropic bandwidth analysis. They make the pure kernel weights consistent, which appear in the Nadaraya-Watson estimator (LPS of order Q = 0) (Györfi et al., 2002, Theorem 5.1 and 5.4). When considering LPS of higher order, it was shown that the *local linear weight function* can be trimmed, relative to the pure kernel weights, in order to make them consistent (Stone, 1977, Corollary 4). In case of non-isotropic bandwidths, a bound on the conditioning number is additionally required to make the local linear weight function bounded: For an unbounded weight function, trimming would lead to predictions that are arbitrarily off the LPS model.

**Remark E2.** For a specific regression task, when searching for LOB over the unbounded set S, it will occur that for a sequence of optimizers  $\Sigma_x^n$  of  $MSE_1(x, \Sigma | \mathbf{X}_n)$ , it is  $\|\Sigma_x^n\|$ ,  $\neq 0$  or even  $\|\Sigma_x^n\| \to \infty$ . To see this, consider  $\Sigma^n = n\mathcal{I}_d$ . Then the LLS predictor  $m_1^{\Sigma^n}$  asymptotically becomes a global linear fit to f. Necessarily,  $\mathbb{E}\left[m_1^{\Sigma^n}(\cdot)|\mathbf{X}_n\right]$  intersects the function f in some  $x \in \mathcal{X}^\circ$ . If it would not, we could shift the offset until the linear fit touches f, by which we reduce the MSE everywhere over  $\mathcal{X}$ . In particular, this means that there always exists some  $x \in \mathcal{X}^\circ$  where LLS is totally free of bias for  $\Sigma^n = n\mathcal{I}_d$ . Hence,  $MSE_1(x, n\mathcal{I}_d | \mathbf{X}_n) = O_p\left[n^{-1}\right]$  at a rate that is superior to any bandwidth sequence with  $\|\Sigma_x^n\| \to 0$ .

This consistency assumption is also made in the related work, when analyzing the isotropic and the non-isotropic, definite cases. Recall that there, in addition, a non-vanishing leading bias-term is required. This requirement enables an explicit construction of LOB, which particularly answers the question of the existence (and uniqueness) of a minimizer. In contrast, in the indefinite case it will turn out that no explicit construction of LOB is possible. Yet, we are able to prove the existence of a minimizer by assuming certain pointwise regularity of the problem. For convenience, recall from (B.4) the space of consistent sequences

$$\mathfrak{S} = \left\{ (\Sigma^n)_{n \in \mathbb{N}} \subset \mathcal{S} \mid |\Sigma^n|^{-1} n^{-1} \to 0, \|\Sigma^n\| \to 0, \|\Sigma^n\| \cdot \|[\Sigma^n]^{-1}\| \le \mathcal{M} \right\}.$$

In order to prove Theorem B7, we will first show in Lemma E3 that there exists an optimal sequence  $(\Sigma_x^n)_{n\in\mathbb{N}} \in \mathfrak{S}$ , for which  $\mathrm{MSE}_1(x, \Sigma_x^n | \mathbf{X}_n) = \Omega_p \left[ n^{-\frac{2\alpha}{2\alpha+d}} \right]$  must necessarily hold. Then we show in Lemma E4 that we are able to construct a sequence  $(\Sigma_x^n)_{n\in\mathbb{N}} \in \mathfrak{S}$  such that  $\mathrm{MSE}_1(x, \Sigma_x^n | \mathbf{X}_n) = O_p \left[ n^{-\frac{2\alpha}{2\alpha+d}} \right]$ .

**Lemma E3** (Minimizer Existence). Let  $x \in \mathcal{X}^{\circ}$  such that f is indefinite in x and for  $\alpha := \alpha(f, x)$  it is  $2 < \alpha < \infty$ . Furthermore assume that v is continuous in x and  $p \in \Lambda^{\alpha-2}(x)$  with p(x), v(x) > 0. Then, there exists  $(\Sigma_x^n)_{n \in \mathbb{N}} \in \mathfrak{S}$  and  $N_x \in \mathbb{N}$  such that for all  $(\Sigma^n)_{n \in \mathbb{N}} \in \mathfrak{S}$ , if  $n \ge N_x$ , it holds that

$$MSE_1(x, \Sigma_x^n | \mathbf{X}_n) \le MSE_1(x, \Sigma^n | \mathbf{X}_n).$$

For such a sequence,  $MSE_1(x, \Sigma_x^n | \mathbf{X}_n) = \Omega_p \left[ n^{-\frac{2\alpha}{2\alpha+d}} \right]$  must hold.

*Proof.* For an arbitrary sequence  $(\Sigma^n)_{n \in \mathbb{N}} \in \mathfrak{S}$  that fulfills the consistency condition in Definition E1, let  $h_n = \|\Sigma^n\|$  and  $\bar{\Sigma}^n = h_n^{-1}\Sigma^n$ . Since  $\alpha(f, x) < \infty$  and  $\|\Sigma^n\| \to 0$  as  $n \to \infty$ , it follows for the bias in x that

$$\mathbb{B}_1[x, \Sigma^n | \boldsymbol{X}_n] = \Omega_p\left[ \|\Sigma^n\|^{\alpha} \right].$$

Hence, we can write

$$\mathbb{B}_1\left[x, \Sigma^n | \boldsymbol{X}_n\right]^2 \ge C(\bar{\Sigma}^n) h_n^{2\alpha} + o_p\left[h_n^{2\alpha}\right],$$

where  $0 < \epsilon_x \leq C(\bar{\Sigma}^n)$ . The lower bound  $\epsilon_x$  exists uniformly for any bandwidth sequence: If not, we could construct  $(\Sigma_n)_{n\in\mathbb{N}} \in \mathfrak{S}$  with  $C(\bar{\Sigma}^n) \to 0$ , for which, in particular,  $\mathbb{B}_1[x, \Sigma^n | \mathbf{X}_n]^2 = o_p \left[ \|\Sigma^n\|^{\alpha} \right]$ , in contradiction to  $\mathbb{B}_1[x, \Sigma^n | \mathbf{X}_n] = \Omega_p \left[ \|\Sigma^n\|^{\alpha} \right]$ .

On the other hand, due to the consistency condition in Definition E1, it is

$$h_n^d = \|\Sigma^n\|^d \ge |\Sigma^n| \ge \|\Sigma^n\| / \|[\Sigma^n]^{-1}\|^{d-1} \ge h_n^d \mathcal{M}^{d-1},$$

such that with  $\mathbb{V}_1[x, \Sigma^n | \mathbf{X}_n] = \frac{R(k)v(x)}{p(x)n|\Sigma^n|} + o_p\left[n^{-1} |\Sigma^n|^{-1}\right]$  it is

$$\frac{R(k)v(x)}{p(x)nh_n^d} \le \mathbb{V}_1\left[x, \Sigma^n | \boldsymbol{X}_n\right] + o_p\left[n^{-1}h_n^d\right] \le \frac{R(k)v(x)}{p(x)nh_n^d \mathcal{M}^{d-1}}$$

Therefore  $\mathbb{V}_1\left[x,\Sigma^n|\boldsymbol{X}_n\right]=\theta_p\left[n^{-1}h_n^{-d}\right],$  such that

$$MSE_{1}(x, \Sigma^{n} | \boldsymbol{X}_{n}) = \mathbb{B}_{1}[x, \Sigma^{n} | \boldsymbol{X}_{n}]^{2} + \mathbb{V}_{1}[x, \Sigma^{n} | \boldsymbol{X}_{n}]$$
  

$$\geq C(\bar{\Sigma}^{n})h_{n}^{2\alpha} + \theta_{p}[n^{-1}h_{n}^{-d}] + o_{p}[h_{n}^{2\alpha} + n^{-1}h_{n}^{-d}]$$
  

$$\geq \epsilon_{x}h_{n}^{2\alpha} + \theta_{p}[n^{-1}h_{n}^{-d}] + o_{p}[h_{n}^{2\alpha} + n^{-1}h_{n}^{-d}].$$

For this lower bound of the MSE, the optimal decay rate is given by  $\underline{h}_n = n^{-\frac{1}{2\alpha+d}}$ . Note that the last claim of the lemma directly follows, since  $\text{MSE}_1(x, \Sigma^n | \boldsymbol{X}_n) = \Omega_p \left[\underline{h}_n^{2\alpha}\right] = \Omega_p \left[n^{-\frac{2\alpha}{2\alpha+d}}\right]$ .

$$\begin{split} & \overset{-n}{\mathrm{MSE}}_{1}\left(x,\Sigma^{n}|\boldsymbol{X}_{n}\right)=\Omega_{p}\left[\underline{h}_{n}^{2\alpha}\right]=\Omega_{p}\left[n^{-\frac{2\alpha}{2\alpha+d}}\right].\\ & \mathrm{Let} \text{ us now define by }\gamma=\frac{1}{2\alpha+d+1}>0 \text{ a strict lower bound on the bandwidth decay exponent. The larger the bias is, the faster an optimal bandwidth sequence has to decay: Since <math>\mathbb{B}_{1}\left[x,\Sigma^{n}|\boldsymbol{X}_{n}\right]=\Omega_{p}\left[\|\Sigma^{n}\|^{\alpha}\right]$$
, let us assume without loss of generality that  $\mathbb{B}_{1}\left[x,\Sigma^{n}|\boldsymbol{X}_{n}\right]=\theta_{p}\left[\|\Sigma^{n}\|^{\beta}\right]$  for some  $\beta\leq\alpha$ . Then, the optimal decay rate becomes  $h_{n}^{*}=n^{-\frac{1}{2\beta+d}}=O_{p}\left[\underline{h}_{n}\right]=o_{p}\left[n^{-\gamma}\right]. We can therefore narrow down the optimal bandwidth candidates to the sets \end{split}$ 

$$S_n = \left\{ \Sigma \in \mathcal{S} \mid \|\Sigma\| \le n^{-\gamma}, |\Sigma| \ge n^{-1} \right\}.$$

On the one hand, the sets  $S_n$  are compact. Using that  $MSE_1(x, \Sigma | X_n)$  is continuous in  $\Sigma \in S$ , there exists  $\Sigma_x^n \in S_n$  such that

$$\operatorname{MSE}_{1}(x, \Sigma_{x}^{n} | \boldsymbol{X}_{n}) = \min_{\Sigma \in S_{n}} \operatorname{MSE}_{1}(x, \Sigma | \boldsymbol{X}_{n}).$$

On the other hand, any sequence that asymptotically resides outside of  $S_n$ , is necessarily suboptimal or not consistent. In this regard, consider any sequence  $(\Sigma^n)_{n \in \mathbb{N}} \in \mathfrak{S}$ . Then

$$\liminf_{n \to \infty} \mathrm{MSE}_1(x, \Sigma^n | \boldsymbol{X}_n) - \mathrm{MSE}_1(x, \Sigma^n_x | \boldsymbol{X}_n) \ge 0.$$

**Lemma E4** (Achievable Rate). Let  $S \subseteq \mathbb{S}_{++}^d$  be conic with  $\dim(S) \geq 2$ . Let  $x \in \mathcal{X}^\circ$  where for  $\alpha := \alpha(f, x)$  it holds that  $2 < \alpha < \infty$  and write  $\alpha = L + \beta$  with  $L \in \mathbb{N}, L \geq 2$  and  $\beta \in (0, 1]$ . Furthermore assume that  $k \in C^{\lfloor L/2 \rfloor}(\mathbb{R}_+, \mathbb{R}_+)$ , v is continuous in x and  $p \in \Lambda^{\alpha-2}(x)$  with p(x), v(x) > 0. If f is indefinite in x, there exists a sequence  $(\Sigma_x^n)_{n \in \mathbb{N}} \in \mathfrak{S}$  such that with  $h_n = n^{-\frac{1}{2\alpha+d}}$ ,

$$MSE_1\left(x, \Sigma_x^n | \boldsymbol{X}_n\right) = O_p\left[h_n^{2\alpha}\right] = O_p\left[n^{-\frac{2\alpha}{2\alpha+d}}\right].$$

*Proof.* Recall the vanishing set of the second-order bias, given by

$$\mathcal{T}_1^x = \left\{ \Sigma \in \mathcal{S} \mid \text{bias}_{1,2} \left[ x, \Sigma \right] = 0 \right\} = \left\{ \Sigma \in \mathcal{S} \mid trace(D_f^2(x)\Sigma^2) = 0 \right\},\$$

and let  $\Sigma_x \in \mathcal{T}_1^x$  be fixed. We will show that for n large enough there always exists  $\Sigma_x^n \in \mathcal{S}$  close to  $\Sigma_x$  such that with  $h_n \to 0$  we will have  $\mathbb{B}_Q(x, h_n \Sigma_x^n | \mathbf{X}_n) = O_p[h_n^{\alpha}]$ :

Let  $l = \lfloor L/2 \rfloor$ . For  $E_n \in \mathbb{S}^d$  we define  $\Sigma_x^n = \Sigma_x + E_n$ . Letting  $\varepsilon_n := ||E_n||$ it is  $\Sigma_x^n \in \mathbb{S}_{++}^d$  for  $\varepsilon_n$  small enough.

Assuming  $h_n, \varepsilon_n \to 0$ , and using the differentiability of the kernel k, we can expand

$$\mathbb{B}_{1}\left[x,h_{n}\Sigma_{x}^{n}|\boldsymbol{X}_{n}\right] = \mathbb{B}_{1}\left[x,h_{n}\Sigma_{x}|\boldsymbol{X}_{n}\right] + \sum_{l=1}^{\lfloor L/2 \rfloor}\sum_{k=1}^{m} b_{1,2l,k}(x,h_{n}\Sigma_{x},E_{n}) + O_{p}\left[h_{n}^{\alpha}\right],$$

where we aggregate with  $b_{1,2l,k}(x, h_n \Sigma_x, E_n) = \theta_p [h_n^{2l} \varepsilon_n^k]$  all terms of the respective order that may appear. It was

$$\mathbb{B}_{1}\left[x, h_{n} \Sigma | \boldsymbol{X}_{n}\right] = \sum_{l=1}^{\lfloor L/2 \rfloor} \operatorname{bias}_{1,2l}\left[x, h_{n} \Sigma\right] + O_{p}\left[h_{n}^{\alpha}\right],$$

where we have by  $\Sigma_x \in \mathcal{T}_1^x$  that the first term  $\operatorname{bias}_{1,2}[x, h_n \Sigma_x] = 0$ . We now separate all terms into two groups as follows:

$$t_1^n(E_n) = \sum_{k=1}^m b_{1,2,k}(x, h_n \Sigma_x, E_n)$$

and

$$t_{2}^{n}(E_{n}) = \sum_{l=2}^{\lfloor L/2 \rfloor} \left[ \operatorname{bias}_{1,2l} \left[ x, h_{n} \Sigma \right] + \sum_{k=1}^{m} b_{1,2l,k}(x, h_{n} \Sigma_{x}, E_{n}) \right].$$

Therefore we have  $\mathbb{B}_1[x, h_n \Sigma_x^n | \boldsymbol{X}_n] = t_1^n(E_n) + t_2^n(E_n) + O_p[h_n^{\alpha}].$ 

- 1. if  $\varepsilon_n \to 0$ , then  $sgn(t_2^n(E_n))$  does not depend on  $sgn(E_n)$ . This is because the leading term of  $t_2^n(E_n)$  is  $bias_{1,4}[x, h_n \Sigma] = O_p[h_n^4]$  in this case.
- 2. There exists  $E \in \mathbb{S}^d$  such that  $\Sigma_x \pm E \in \mathbb{S}^d_{++}$  and  $sgn(t_1^n(E_n)) = \pm 1$
- 3.  $t_1^n(\lambda E) \to 0$  as  $\lambda \to 0$ .
- 4. For fixed  $E_n \equiv E$  with  $\Sigma_x^n = \Sigma_x + E$  it is  $t_1^n(E) = \theta_p \left[h_n^2\right]$ , whereas  $t_2^n(E) = O_p \left[h_n^4\right]$ .

Because of (1) and (2), we can choose  $sgn(t_1^n) = -sgn(t_2^n)$  for n large enough. When plugging in the E from (2) in (4), for n large enough  $|t_2^n(E)| \leq |t_1^n(E)|$ . When we increase n beyond that, we find  $\lambda_n \in (0,1)$  with (3) such that  $|t_2^n(\lambda_n E)| \equiv |t_1^n(\lambda_n E)|$ . Here it is necessarily  $\lambda_n = O_p[\varepsilon_n] \to 0$ . Now, with  $E_n = \lambda_n E$  and  $|t_2^n(E_n)| \equiv |t_1^n(E_n)|$  and  $sgn(t_1^n(E_n)) = -sgn(t_2^n(E_n))$ , it follows  $t_1^n(E_n) + t_2^n(E_n) \equiv 0$  such that

$$\mathbb{B}_1\left[x, h_n \Sigma_x^n | \boldsymbol{X}_n\right] = t_1^n(E_n) + t_2^n(E_n) + O_p\left[h_n^\alpha\right] = O_p\left[h_n^\alpha\right].$$

Note that, since  $t_1^n(E_n) = O_p \left[h_n^2 \varepsilon_n\right]$ ,  $t_2^n(E_n) = O_p \left[h_n^4\right]$  and  $t_1^n(E_n) + t_2^n(E_n) \equiv 0$ , it is necessarily  $\varepsilon_n = O_p \left[h_n^2\right]$ . Furthermore, with  $\mathbb{V}_1 \left[x, h_n \Sigma_x^n | \mathbf{X}_n\right] = \mathbb{V}_1 \left[x, h_n \Sigma_x | \mathbf{X}_n\right] (1 + O_p \left[\varepsilon_n\right]) = O_p \left[h_n^{-d} n^{-1}\right]$  it is

$$MSE_1(x, h_n \Sigma_x^n | \boldsymbol{X}_n) = \mathbb{B}_1 [x, h_n \Sigma_x^n | \boldsymbol{X}_n]^2 + \mathbb{V}_1 [x, h_n \Sigma_x^n | \boldsymbol{X}_n] = O_p \left[ h_n^{2\alpha} + h_n^{-d} n^{-1} \right].$$

With the optimal trade-off, being  $h_n = n^{-\frac{1}{2\alpha+d}}$ , it is therefore

$$\mathrm{MSE}_{1}\left(x,h_{n}\Sigma_{x}^{n}|\boldsymbol{X}_{n}\right)=O_{p}\left[h_{n}^{2\alpha}\right]=O_{p}\left[n^{-\frac{2\alpha}{2\alpha+d}}\right]$$

as claimed.

In the light of Lemma E3, the bandwidth sequence from Lemma E4 is rate-optimal, such that up to a constant, no better result can be obtained with the LLS model class, using a consistent bandwidth sequence.

**Theorem B7** (Non-isotropic LOB and MSE of LLS for indefinite functions). Let  $S = \mathbb{S}_{++}^d$  with  $d \ge 2$ . Let  $x \in \mathcal{X}^\circ$  where for  $\alpha := \alpha(f, x)$  it holds that  $2 < \alpha < \infty$  and write  $\alpha = L + \beta$  with  $L \in \mathbb{N}, L \ge 2$  and  $\beta \in (0, 1]$ . Furthermore assume that  $k \in C^{\lfloor L/2 \rfloor}(\mathbb{R}_+, \mathbb{R}_+)$ , v is continuous in x and  $p \in \Lambda^{\alpha-2}(x)$  with p(x), v(x) > 0. If f is indefinite in x, then there exists a sequence  $(\Sigma_x^n)_{n \in \mathbb{N}} \in \mathfrak{S}$  such that with  $h_n = n^{-\frac{1}{2\alpha+d}}$ ,

$$MSE_1(x, \Sigma_x^n | \mathbf{X}_n) = \theta_p \left[ h_n^{2\alpha} \right] = \theta_p \left[ n^{-\frac{2\alpha}{2\alpha+d}} \right],$$

and  $N_x \in \mathbb{N}$  such that for all  $(\Sigma^n)_{n \in \mathbb{N}} \in \mathfrak{S}$ , if  $n \geq N_x$ , it holds that

$$MSE_1(x, \Sigma_x^n | \mathbf{X}_n) \le MSE_1(x, \Sigma^n | \mathbf{X}_n).$$

For such a sequence,  $\Sigma_x^n = \theta_p \left[ n^{-\frac{1}{2\alpha+d}} \mathbb{1}_d \mathbb{1}_d^\top \right]$  and  $\inf_{\Sigma \in \mathcal{T}_1^x} \|h_n^{-1} \Sigma_x^n - \Sigma\| = O_p \left[ h_n^2 \right]$  must hold.

*Proof.* The claim immediately follows from combining Lemma E3 and E4.

## Appendix F. The reciprocal determinant of non-isotropic LOB of LLS for indefinite functions

Recall that we know nothing about its uniqueness of LOB in the indefinite regime, for which reason we have introduced the set-valued definition (B.5) of LOB via

$$\Sigma_{1,\mathbb{S}_{++}^d}^n(x) = \{ \Sigma \in S_n \mid \mathrm{MSE}_1(x, \Sigma | \boldsymbol{X}_n) = \min_{\Sigma' \in S_n} \mathrm{MSE}_1(x, \Sigma' | \boldsymbol{X}_n) \}.$$

We will now show that, for  $\Sigma_n, \Sigma'_n \in \Sigma_{1,\mathbb{S}^d_{++}}^n(x)$  with  $\Sigma_n \neq \Sigma'_n$  it is  $|h_n^{-1}\Sigma_n| - |h_n^{-1}\Sigma'_n| = o_p[1]$ , where  $h_n = n^{-\frac{1}{2\alpha+d}}$ . So with abuse of notation,  $x \mapsto |h_n^{-1}\Sigma_{1,\mathbb{S}^d_{++}}^n(x)|$  is an asymptotically well-defined function over the input space. First of all note that we can generalize the balancing property in Corollary 8 to the non-isotropic case:

**Lemma F1.** May the assumptions of Theorem B7 hold and let  $(\Sigma_n^x)_{n \in \mathbb{N}} \in \mathfrak{S}$ be an optimal bandwidth sequence in  $x \in \mathcal{X}^\circ$ . That is,  $\Sigma_x^n \in \Sigma_{1,\mathbb{S}_{++}^d}^n(x)$ . The conditional bias can be expressed through the conditional variance as

$$\mathbb{B}_1[x, \Sigma_x^n | \boldsymbol{X}_n]^2 = \frac{d}{2\alpha} var_1[x, \Sigma_x^n | \boldsymbol{X}_n] + o_p \left[ n^{-\frac{2\alpha}{2\alpha+d}} \right].$$

Hence the conditional MSE can asymptotically be expressed as

$$MSE_1\left(x, \Sigma_x^n | \boldsymbol{X}_n\right) = \frac{2\alpha + d}{2\alpha} var_1\left[x, \Sigma_x^n | \boldsymbol{X}_n\right] + o_p\left[n^{-\frac{2\alpha}{2\alpha + d}}\right].$$
 (F.1)

*Proof.* For the optimal decay rate  $h_n = n^{-\frac{1}{2\alpha+d}}$  define  $\bar{\Sigma}_x^n := h_n^{-1} \Sigma_x^n$ . Let us write  $\mathbb{B}_1 [x, \Sigma_x^n | \mathbf{X}_n]^2 = C(\bar{\Sigma}_x^n) h_n^{2\alpha} + o_p [h_n^{2\alpha}]$  such that

$$\mathrm{MSE}_1\left(x,h_n\bar{\Sigma}^n_x|\boldsymbol{X}_n\right) = C(\bar{\Sigma}^n_x)h_n^{2\alpha} + \frac{R(k)v(x)}{h_n^d|\bar{\Sigma}^n_x|p(x)n} + o_p\left[h_n^{2\alpha} + n^{-1}h_n^{-d}\right].$$

Necessarily,  $C(\bar{\Sigma}_x^n) \not\rightarrow \infty$  and  $|\bar{\Sigma}_x^n| \not\rightarrow 0$  since else  $\text{MSE}_1(x, h_n \bar{\Sigma}_x^n | \mathbf{X}_n) = \omega_p \left[h_n^{2\alpha}\right]$ , contradicting the optimality of the sequence. On the other hand,  $C(\bar{\Sigma}_x^n) \not\rightarrow 0$  and  $|\bar{\Sigma}_x^n| \not\rightarrow \infty$  as we could else adjust  $h_n$  accordingly, which results in a MSE convergence rate faster than the optimal rate. Therefore both sequences,  $C(\bar{\Sigma}_x^n)$  and  $|\bar{\Sigma}_x^n|$ , have at least one accumulation point. Without loss of generality, we assume  $C(\bar{\Sigma}_x^n) \rightarrow C$  and  $|\bar{\Sigma}_x^n| \rightarrow A$ , since the result holds true for any subsequence converging to an arbitrary combination of accumulation points.

The optimal  $h_n$  can be found by setting the derivative of the leading error terms to zero:

$$\begin{split} 0 &= \frac{\partial}{\partial h_n} \mathrm{MSE}_1\left(x, h_n \bar{\Sigma}_x^n | \boldsymbol{X}_n\right) = 2\alpha C h_n^{2\alpha - 1} - \frac{dR(k)v(x)}{h_n^{d+1} A p(x)n} \\ \Leftrightarrow h_n^{2\alpha + d} &= \frac{dR(k)v(x)}{2\alpha C A p(x)n}. \end{split}$$

However, since  $\Sigma_x^n = h_n \overline{\Sigma}_x^n$  is optimal for  $h_n = n^{-\frac{1}{2\alpha+d}}$ , it already must hold

$$\frac{dR(k)v(x)}{2\alpha CAp(x)} = 1 \Leftrightarrow C = \frac{dR(k)v(x)}{2\alpha Ap(x)}.$$

Therefore

$$\begin{split} \mathbb{B}_1 \left[ x, \Sigma_x^n | \boldsymbol{X}_n \right]^2 + o_p \left[ h_n^{2\alpha} \right] \\ = h_n^{2\alpha} C = h_n^{2\alpha} \frac{dR(k)v(x)}{2\alpha A p(x)} = \frac{d}{2\alpha} \operatorname{var}_1 \left[ x, \Sigma_x^n | \boldsymbol{X}_n \right] + o_p \left[ h_n^{2\alpha} \right], \end{split}$$

such that

$$MSE_1(x, \Sigma_x^n | \boldsymbol{X}_n) = \frac{2\alpha + d}{2\alpha} \operatorname{var}_1[x, \Sigma_x^n | \boldsymbol{X}_n] + o_p[h_n^{2\alpha}].$$

From this, we can deduce the asymptotic uniqueness of the reciprocal determinant of  $\sum_{1,\mathbb{S}_{+\perp}^d}^n (x)$ :

**Corollary F2.** May the assumptions of Theorem B7 hold for  $x \in \mathcal{X}^{\circ}$ . Furthermore let  $(\Sigma_n)_{n \in \mathbb{N}}, (\Sigma'_n)_{n \in \mathbb{N}} \in \mathfrak{S}$  be two consistent, optimal bandwidth sequences. That is,  $\Sigma_n, \Sigma'_n \in \Sigma^n_{1, \mathbb{S}^d_{++}}(x)$ . Then

$$|h_n^{-1}\Sigma_n|^{-1} = |h_n^{-1}\Sigma_n'|^{-1} + o_p[1].$$

*Proof.* It holds  $MSE_1(x, \Sigma_n | \mathbf{X}_n) = MSE_1(x, \Sigma'_n | \mathbf{X}_n) + o_p[h_n^{2\alpha}]$  due to the optimality of both sequences, such that according to Lemma F1 it is

$$\frac{2\alpha+d}{2\alpha}\frac{R(k)v(x)}{\left|\Sigma_{n}\right|p(x)n}+o_{p}\left[h_{n}^{2\alpha}\right]=\frac{2\alpha+d}{2\alpha}\frac{R(k)v(x)}{\left|\Sigma_{n}'\right|p(x)n}+o_{p}\left[h_{n}^{2\alpha}\right].$$

Therefore

$$[n |\Sigma_n|]^{-1} = [n |\Sigma'_n|]^{-1} + o_p [h_n^{2\alpha}] \Leftrightarrow |h_n^{-1}\Sigma_n|^{-1} = |h_n^{-1}\Sigma'_n|^{-1} + o_p [1]$$

From here on, we can treat  $D_n(x) = \left| h_n^{-1} \Sigma_{1,\mathbb{S}_{++}^d}^n(x) \right|$  as a function that is asymptotically well-defined. This family of functions features pointwise convergence:

**Lemma F3.** There exists a function  $D: \mathcal{X} \to \mathbb{R}_{++}$  such that

$$D_n(x) = D(x) + o_p[1].$$
 (F.2)

*Proof.* Let us do the following preliminary consideration: At (sampling-)time n we regard  $x_{n+1}$  as close to x, relative to  $\sum_{1,\mathbb{S}_{++}^d}^n (x)$ , if  $\|\sum_{1,\mathbb{S}_{++}^d}^n (x)^{-1}(x - x_{n+1})\| \leq s$ , where it is [0,s] the support of the kernel k. Let therefore  $p_n = \mathbb{P}\{x_{n+1} \text{ is close to } x'\} = c \left|\sum_{1,\mathbb{S}_{++}^d}^n (x)\right|$  for some adequate constant c > 0. Note that  $p_n = O_p \left[h_n^d\right]$ . Furthermore let  $D_n(x)$  be known and fixed.

Now, if  $x_{n+1}$  is not close to x, then  $x_{n+1}$  has no influence on the MSE and LOB in x. Thus,  $\sum_{1,\mathbb{S}_{++}^d}^{n+1}(x) = \sum_{1,\mathbb{S}_{++}^d}^n(x)$  such that

$$D_{n+1}(x) = \left| h_{n+1}^{-1} \Sigma_{1,\mathbb{S}_{++}^d}^{n+1}(x) \right|^{-1} = \frac{h_{n+1}^d}{h_n^d} \left| h_n^{-1} \Sigma_{1,\mathbb{S}_{++}^d}^n(x) \right|^{-1} = \left[ \frac{n}{n+1} \right]^{\frac{d}{2\alpha+d}} D_n(x)$$

If  $x_{n+1}$  is close to x, then it has an influence on LOB in x, which is proportional to the effective sample size  $N_n(x) := nc' \left| \sum_{1, \mathbb{S}_{++}^d}^n (x) \right|$  in x at time n, for some adequate constant c' > 0. In particular, the effective sample size grows as

$$N_{n+1}(x) = N_n(x) + 1 = (n + [c' \left| \sum_{1, \mathbb{S}_{++}^d}^n (x) \right|]^{-1})c' \left| \sum_{1, \mathbb{S}_{++}^d}^n (x) \right|.$$

In summary, the event that  $x_{n+1}$  is not close to x leads to a decrease of  $D_{n+1}(x)$ , whereas  $x_{n+1}$  is close to x will in general lead to an increase of  $D_{n+1}(x)$ . Additionally, as n grows, the per-sample impact on  $D_n(x)$  decreases in both directions.

Like in the proof of Lemma F1, we know that  $D_n(x)$  is a sequence that is bounded in probability: If not, then the bandwidth sequence  $\sum_{1,\mathbb{S}_{++}^d}^n (x)$  would lead to a decay-law of the MSE that is different to the optimal  $O_p[h_n^{2\alpha}]$ , which either contradicts the optimality of this decay-law or the optimality of the bandwidth sequence itself. Therefore there exist  $0 < \underline{D} < \overline{D} < \infty$ , which bound  $D_n(x)$  in probability. That is, for all  $\varepsilon > 0$  there exists  $\mathfrak{N} \in \mathbb{N}$  such that for all  $n \geq \mathfrak{N}$ :

$$\mathbb{P}(\underline{D} \le D_n(x) \le \overline{D}) > 1 - \varepsilon$$

Now, if D(x) would not exist for which  $D_n(x) = D(x) + o_p[1]$  holds, then there exists  $\delta > 0$  such that for any  $0 < \underline{D} < \overline{D} < \infty$ , which bound  $D_n(x)$  in probability, it is  $\overline{D} - \underline{D} \ge \delta$ . Without loss of generality let us choose these bounds such that  $\overline{D} - \underline{D} = \delta$ . Then there exist  $\underline{\varepsilon}, \overline{\varepsilon} > 0$  such that for infinitely many  $n \in \mathbb{N}$  it is

$$\mathbb{P}(D_n(x) \le \underline{D} + \frac{\delta}{4}) \ge \underline{\varepsilon} \text{ and } \mathbb{P}(D_n(x) \ge \overline{D} - \frac{\delta}{4}) \ge \overline{\varepsilon}.$$

In particular, we can construct index sequences  $(n_m)_{n \in \mathbb{N}}, (n'_m)_{n \in \mathbb{N}}$  such that  $n_m < n'_m < n_{m+1}, n_m \to \infty$ , and for all  $m \in \mathbb{N}$ :

$$\mathbb{P}(D_{n_m}(x) \leq \underline{D} + \frac{\delta}{4}) > \underline{\varepsilon} \quad \text{and} \qquad \mathbb{P}(D_{n'_m}(x) \geq \overline{D} - \frac{\delta}{4}) \geq \overline{\varepsilon}.$$

Then, for all  $m \in \mathbb{N}$ ,  $\mathbb{P}(D_{n'_m}(x) - D_{n_{m+1}}(x) > \frac{\delta}{2}) > \underline{\varepsilon}\overline{\varepsilon} =: \tilde{\varepsilon}$ .

We now can choose M > m such that  $\Sigma_1^{n'_m}(x) \ge_L \Sigma_1^{n_M}(x)$  in the sense of the *Loewner* order. That is,  $\Sigma_1^{n'_m}(x) - \Sigma_1^{n_M}(x)$  is positive semi-definite. Then, letting  $N = n'_M - n_M$ , the sampled training inputs

$$x_{n_M+1} := z_1, \dots, x_{n'_M} := z_N$$

lead to an increase from  $D_{n_M}(x)$  to  $D_{n'_M}(x)$  of at least  $\frac{\delta}{2}$  with probability greater than  $\tilde{\varepsilon}$ .

Now that  $\Sigma_1^{n'_m}(x) \geq_L \Sigma_1^{n_M}(x)$ , the samples  $z_1, \ldots, z_N$  are closer to x at time  $n'_m$  than at time  $n_M$ . Therefore, when observing

$$x_{n'_m+1} = z_1, \dots, x_{n'_m+N} = z_N$$

at this earlier point-in-time, when moving from  $D_{n'_m}(x)$  to  $D_{n'_m+N}(x)$ , we would encounter at least the same amount of samples – if not more – that lead to an increase. Combining this with the fact that the per-sample fluctuations are stronger at time  $n'_m$  than at  $n_M$ , it is

$$\mathbb{P}(D_{n'_m+N}(x) - D_{n'_m}(x) \ge \frac{\delta}{2}) \ge \mathbb{P}(D_{n'_M}(x) - D_{n_M}(x) \ge \frac{\delta}{2}) > \tilde{\varepsilon}.$$

Since it was  $\mathbb{P}(D_{n'_m}(x) \ge \overline{D} - \frac{\delta}{4}) \ge \underline{\varepsilon}$ , it follows

$$\mathbb{P}(D_{n'_m+N}(x) \ge \overline{D} + \frac{\delta}{4})$$
  
$$\ge \mathbb{P}(D_{n'_m}(x) \ge \overline{D} - \frac{\delta}{4}, D_{n'_m+N}(x) - D_{n'_m}(x) \ge \frac{\delta}{2}) \ge \underline{\varepsilon}\tilde{\varepsilon} =: \epsilon > 0$$

Finally, for any  $\mathfrak{N} \in \mathbb{N}$  we can choose  $m \geq \mathfrak{N}, M > m$  and  $N = n'_M - n_M$  such that, respectively,  $n'_m + N > \mathfrak{N}$  with  $\mathbb{P}(D_{n'_m + N}(x) \geq \overline{D} + \frac{\delta}{4}) > \epsilon$ . This is in contradiction to the choice of  $\overline{D}$  as an upper bound of  $D_n(x)$  in probability. We will assume from now on, that  $f \in \mathcal{C}^{\alpha}(\mathcal{X})$ , and furthermore, that  $\alpha(f, x) \equiv \alpha$  for all  $x \in \mathcal{X}^{\circ}$ . In this case, we can choose the functions  $D_n$  to be continuous.

**Lemma F4** (Continuity). Let  $f \in C^{\alpha}(\mathcal{X})$  and may the assumptions of Theorem B7 hold uniformly with  $\alpha(f, x) \equiv \alpha$  for all  $x \in \mathcal{X}^{\circ}$ . Then there exist  $D_n \in C^0(\mathcal{X}, \mathbb{R}_{++})$  such that

$$\left|h_n^{-1}\Sigma_{1,\mathbb{S}_{++}^d}^n(x)\right|^{-1} = D_n(x) + o_p[1],$$

almost everywhere in  $\mathcal{X}$ .

*Proof.* From the proof of Lemma E3 we know that for  $\gamma = \frac{1}{2\alpha + d + 1} > 0$ , we can bound  $\|\Sigma_x^n\| \leq n^{-\gamma}$  and  $|\Sigma_x^n| \geq \frac{1}{n}$  for almost every  $x \in \mathcal{X}^{\circ}$ , n large enough and  $\Sigma_x^n \in \Sigma_{1,\mathbb{S}_{++}^d}^n(x)$ . Let

$$S_n = \left\{ \Sigma \in \mathcal{S} \mid \|\Sigma\| \le n^{-\gamma}, |\Sigma| \ge n^{-1} \right\},\$$

and recall that  $S_n$  is compact. Using that  $MSE_1(x, \Sigma | X_n)$  is continuous in both,  $x \in \mathcal{X}$  and  $\Sigma \in \mathcal{S}$ , it generally holds that

$$x \mapsto \min_{\Sigma \in S_n} \mathrm{MSE}_1(x, \Sigma | \boldsymbol{X}_n) \in \mathcal{C}^0(\mathcal{X}, \mathbb{R}_{++}).$$

is a continuous function over the input space. Note that, for n large enough,

$$\operatorname{MSE}_{1}(x, \Sigma_{x}^{n} | \boldsymbol{X}_{n}) = \min_{\Sigma \in S_{n}} \operatorname{MSE}_{1}(x, \Sigma | \boldsymbol{X}_{n})$$

and, according to Lemma F.1, that

$$MSE_{1}(x, \Sigma_{x}^{n} | \boldsymbol{X}_{n}) = \frac{2\alpha + d}{2\alpha} \operatorname{var}_{1}[x, \Sigma_{x}^{n} | \boldsymbol{X}_{n}] + o_{p}[h_{n}^{2\alpha}] = \frac{2\alpha + d}{2\alpha} \frac{R(k)v(x)}{|\Sigma_{z}^{n}| p(x)n} + o_{p}[h_{n}^{2\alpha}]$$

When rearranging terms, it is

$$\left|h_n^{-1}\Sigma_x^n\right|^{-1} = \underbrace{h_n^{-2\alpha}\text{MSE}_1\left(x,\Sigma_x^n|\boldsymbol{X}_n\right)\frac{2\alpha}{2\alpha+d}\frac{p(x)}{R(k)v(x)}}_{=:D_n^{\circ}(x)} + o_p\left[1\right].$$

With all functions,  $MSE_1(x, \Sigma_x^n | \mathbf{X}_n)$ , p(x) and v(x), being continuous in x, it follows that  $D_n^{\circ}(x)$  – as defined above – is continuous in x. Now that the above proof holds true for almost every  $x \in \mathcal{X}^{\circ}$ , the function  $D_n^{\circ}$  is well-defined and continuous, almost everywhere in  $\mathcal{X}^{\circ}$ . Finally, the closure of  $D_n^{\circ}$  in  $\mathcal{X}$ , given by

$$D_n(x) = \lim_{z \in \mathcal{X}^\circ, z \to x} D_n^\circ(z),$$

is continuous and fulfills via construction almost everywhere

$$\left|h_n^{-1}\Sigma_{1,\mathbb{S}_{++}^d}^n(x)\right|^{-1} = D_n(x) + o_p[1].$$

**Theorem B10.** Let  $f \in C^{\alpha}(\mathcal{X})$  and may the assumptions of Theorem B7 hold uniformly with  $\alpha(f, x) \equiv \alpha$  for all  $x \in \mathcal{X}^{\circ}$ . Then there exist  $D_n \in C^0(\mathcal{X}, \mathbb{R}_{++})$  such that

$$\left| h_n^{-1} \Sigma_{1, \mathbb{S}_{++}^d}^n(x) \right|^{-1} = D_n(x) + o_p \left[ 1 \right],$$

almost everywhere in  $\mathcal{X}$ . Furthermore there exists a limiting function D such that

$$D_n(x) = D(x) + o_p \left[1\right].$$

*Proof.* The claim follows from combining Corollary F2, Lemma F3 and F4.

We now know that  $D_n$  is a family of continuous functions with pointwise limits  $D(x) = \lim_{n \to \infty} D_n(x)$ . But since we are not aware about uniform convergence of  $D_n$ , we cannot imply the continuity of D(x). Yet, we can try to deduce from the scaling behavior of D how to adjust  $D_n$  for the effects of v and p:

Since the bias-component does not depend on the noise level v in general, it is  $D_n(x) \propto v(x)^{-\frac{d}{2\alpha+d}}$  which follows straight-forward to the isotropic case. In contrast, we have seen that higher-order bias-components depend on pthrough its derivatives. Even though it is impossible to construct the true asymptotic bias explicitly in the indefinite regime, it is therefore likely to depend on p in a non-trivial way.

Yet, in case of  $p \sim \mathcal{U}(\mathcal{X})$  this problem does not occur, since all derivatives of p vanish. The same argument will hold for training densities that can be written as step-functions

$$p(x) = \sum_{s=1}^{S} \mathbf{1}_{X_s}(x) P_s,$$

where  $\mathcal{X} = X_1 \uplus \ldots \uplus X_S$  is a partition of the input space with constant density values  $P_s > 0$ .