Distributionally Robust Gaussian Process Regression and Bayesian Inverse Problems

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Abstract

We study a distributionally robust optimization formulation (i.e., a min-max game) for two representative problems in Bayesian nonparametric estimation: Gaussian process regression and, more generally, linear inverse problems. Our formulation seeks the best mean-squared error predictor, in an infinite-dimensional space, against an adversary who chooses the worst-case model in a Wasserstein ball around a nominal infinite-dimensional Bayesian model. The transport cost is chosen to control features such as the degree of roughness of the sample paths that the adversary is allowed to inject. We show that the game has a well-defined value (i.e., strong duality holds in the sense that max-min equals min-max) and that there exists a unique Nash equilibrium which can be computed by a sequence of finite-dimensional approximations. Crucially, the worst-case distribution is itself Gaussian. We explore properties of the Nash equilibrium and the effects of hyperparameters through a set of numerical experiments, demonstrating the versatility of our modeling framework.

1 Introduction

Bayesian nonparametric estimation is used ubiquitously in science, engineering, and other areas of statistical application, both for ‘direct’ nonparametric regression and the solution of inverse problems. The computation of posterior (or conditional) mean estimators, which are the most commonly used Bayesian point estimators, involves the solution of an infinite-dimensional optimization problem, whose specification requires knowledge of the distributions at hand. In general, this problem has no closed-form solution. If the observations and the parameter of interest are jointly Gaussian, however, then the problem immediately becomes tractable. The conditional expectation (the best mean-square estimator of the parameter) is an affine function of the observations. Conditional covariances also can be evaluated easily, enabling some quantification of prediction uncertainty.
Of course, Gaussianity is a strong assumption that is easily violated in reality. More generally, the joint probabilistic model for the parameter of interest and the observations is often—perhaps inevitably—misspecified. This misspecification can take myriad forms, including incorrect prior assumptions on the smoothness or dependence structure of the unknown parameter, and incorrect assumptions on the nature of the data-generating process—which in turn involves assumptions on both the observational noise and, in the inverse problem setting, on the “forward” operator relating the parameters to the observations. In these situations, it is desirable to ensure some form of robustness, e.g., to construct a nonparametric estimator that hedges against the impact of model misspecification on mean-square error. One also would like to represent possible modeling errors nonparametrically, and in way that fully reflects the infinite-dimensional nature of the regression and inverse problem settings.

This paper addresses model misspecification in nonparametric settings, by adapting and extending ideas from distributionally robust optimization (DRO) [6, 14, 28, 23, 11]. DRO formulations create a min-max game between a decision-maker and an adversary, where the latter is introduced to assess the impact of model misspecification on the decision-maker’s chosen criterion. Here, we introduce a DRO formulation for infinite-dimensional Gaussian models. In our formulation, the decision-maker seeks an estimator of the unknown parameter that minimizes a certain Bayes risk, and the adversary chooses a probabilistic model that departs (in a nonparametric way, subject to a budget constraint) from the baseline/nominal Gaussian model assumed by the decision maker. Specifically, we will allow the adversary to select a model within a certain $\delta$-Wasserstein ball around the nominal model. The particular Wasserstein geometry that we impose (to be described precisely below) allows the adversary to select models that depart significantly not only from the Gaussian assumption but also from the smoothness properties dictated by the decision-maker’s choice of prior. Consequently, our min-max formulation allows us to efficiently explore and assess the impact of model misspecification.

To make these ideas concrete, we contrast the nominal and robust estimation problems as follows. (More precise presentations of both problems are deferred to Section 2.) Let $b^0$ represent the parameter of interest, modeled as a real-valued random process with continuous sample paths on some compact domain $D \subseteq \mathbb{R}^d$. Suppose we have a finite number of real-valued observations $(Y_1, \ldots, Y_m)$, specified as $Y_i = T(b^0)(x_i) + \epsilon^0_i$, where $T$ is a bounded linear operator, $(x_i)_{i=1}^m \in D$ are collocation or design points, and $(\epsilon^0_i)_{i=1}^m$ are independent real-valued random variables representing, e.g., observational noise. In the nominal case, $b^0$ and $\epsilon^0_i$ are endowed with a Gaussian prior measure $P_0$ (under which $\epsilon^0_i$ are independent of $b^0$) on $L^2(D) \times \mathbb{R}^m$ and we seek an estimator $\phi : \mathbb{R}^m \to L^2(D)$ that minimizes the Bayes risk

$$
\min_{\phi} \mathbb{E}_{P_0} \left[ \|b^0 - \phi(Y_1, \ldots, Y_m)\|^2_{L^2(D)} \right]. 
$$

(1)

It is well known that this estimator is given by the conditional expectation $\phi(Y_1, \ldots, Y_m) =$
We build the Wasserstein distributionally robust counterpart of this problem by introducing an ambiguity set of probability measures, \( \{ P : W(P, P_0) \leq \delta \} \), where \( W \) is a certain Wasserstein distance on the space of (Borel) probability measures on \( C(D) \times \mathbb{R}^m \). (Our construction of this distance is given in Section 2.2.) We then seek an estimator \( \phi \) that minimizes the worst-case Bayes risk over this ambiguity set:

\[
\inf_{\phi} \sup_{P : W(P, P_0) \leq \delta} \mathbb{E}_P \left[ \| b - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right],
\]

(2)

where now \( Y_i = T(b)(x_i) + \epsilon_i \), and \( b \) and \( \epsilon_1, \ldots, \epsilon_m \) are jointly distributed according to \( P \). The robust formulation thus adds an adversary to the nominal formulation.

By choosing among distributions in the ambiguity set, the adversary may inject additional roughness to sample paths of \( b \), beyond what is allowed by the nominal distribution \( P_0 \). The ability to add roughness is directly tied to our specification of \( W \): we consider perturbations to \( b \) that are elements of an RKHS \( \mathcal{H}_w \) whose norm is parameterized by a sequence of weights \( (w_n)_{n \geq 1} \). Using these weights, the ground cost defining our Wasserstein distance can adjust the penalty for transportation along different “modes” of the spectral decomposition of \( b \). This infinite-dimensional construction is an important novelty from the DRO perspective. The adversary also can modify the distribution of the additive noise \( \epsilon_i \), which can be understood in part as compensating for misspecification of the nominal forward operator \( T \) [18]. Moreover, the adversary can replace \( P_0 \) (in any of its marginals or jointly) with a distribution that is non-Gaussian.

Our requirements on the operator \( T \) in the formulation above will encompass many linear inverse problems [33, 10], e.g., learning the initial or boundary conditions of a heat equation, or canonical problems in computerized tomography [24]. By setting \( T = \text{Id} \), however, we recover the important case of Gaussian process regression, to which our main results immediately apply. For non-identity \( T \), our results apply both to recovering \( b \) (e.g., solving the inverse problem) and to estimating \( u \) (e.g., PDE constrained regression).

Wasserstein-type distances defined on the space of stochastic processes were recently studied by [4, 1, 5]. The focus therein is on processes indexed by a one-dimensional parameter (representing, for instance, time). A typical setting involves price processes in finance [4, 1], where one needs to define a Wasserstein distance that respects causal structure (i.e., filtrations). In contrast, we consider in this work a Wasserstein distance on multi-dimensional fields. Note also that in our formulation (2) we have an infinite-dimensional action space for the outer player and an infinite-dimensional action space for the inner player. Moreover, the actions of the inner player are themselves probability measures on infinite-dimensional spaces. These features differentiate our analysis from prior work, such as [5, [23, 28]. To our knowledge, previous work in the distributionally robust optimization literature assumes either the action set of the decision maker to be finite-dimensional or the probability measures (the action set of the inner player) to be supported on finite-dimensional spaces.
As an alternative, one can naturally formulate problem (2) with the Wasserstein distance being replaced by an information divergence. Distributionally robust conditional mean estimation with a relative entropy ambiguity set centered on a multivariate Gaussian prior has been studied in [20, 21, 39]. As shown in [20, Theorem 1] and [21, Theorem 1], however, the resulting robust estimator coincides exactly with its non-robust counterpart, and only the posterior covariance is inflated. The same conclusion holds for ambiguity sets constructed from the \( \tau \)-divergence family [41, 40]. In strong contrast to these results, the robust estimator of our formulation (2) typically differs from its non-robust counterpart.

While the results just discussed were derived in the finite-dimensional setting, it is reasonable to expect that similar properties of the estimator would be preserved (under reasonable assumptions) in the infinite-dimensional setting, which is our concern here. Distributionally robust formulations of non-causal filtering that employ a relative entropy or \( \tau \)-divergence ambiguity set centered on a stationary Gaussian process prior have been studied in [21, 40], where it was shown that the nominal non-causal Wiener filter remains optimal. Moreover, an infinite-dimensional DRO formulation based on, e.g., relative entropy or any other criterion that requires the existence of a likelihood ratio will typically restrict the adversary to preserve sample path properties, such as the degree of sample path smoothness under the baseline model (i.e., the prior \( P_0 \)). Choosing instead a Wasserstein ambiguity set, as we will explain, permits adversarial distributions with rougher sample paths than the prior, so that smoothness misspecification is naturally addressed by our robust estimation problem.

We now summarize our main contributions. Under reasonable assumptions to be made precise later:

- We analyze problem (2) and show that strong duality holds, in the sense that the minimization and the maximization operators can be switched without any loss of optimality.

- We show that there exists an upper bound \( \delta_0 > 0 \) such that if \( 0 < \delta < \delta_0 \), problem (2) also admits a unique Nash equilibrium pair \( (\phi^*_\infty, P^*_\infty) \). Moreover, the worst case distribution \( P^*_\infty \) involves a modified Gaussian process with potentially rougher paths than the prior. Consequently, the robustified decision remains affine in the observations and the optimization problem is tractable.

- We approximate problem (2) by a sequence of finite-dimensional counterparts and therefore obtain a procedure to compute the associated Nash equilibrium. Our numerical algorithm is an adaptation of the (finite-dimensional) Frank-Wolfe algorithm in [28].

One way to interpret our results is that Gaussian process regression (or the solution of linear inverse problems) can be made robust in a nonparametric sense. The interpretation of the worst-case covariance function (i.e., the covariance of the Gaussian process \( P^*_\infty \)) is then important, as it enables computing a bound on the worst-case mean square error and thus an upper bound on the quality of the robust solution. We explore the structural
properties of this worst-case covariance function, and the associated robust estimator, in our numerical examples. In particular we explore the prior and posterior covariances of \( b \) under \( P_0 \) and \( P^*_\infty \) (i.e., \( \text{Cov}_P[b] \) and \( \text{Cov}_P[b \mid y_1, \ldots, y_m] \) for \( P = P_0 \) and \( P = P^*_\infty \)) and find that the worst-case distributions (both prior and posterior) have greater uncertainty in regions of \( D \) where information is limited, which intuitively guarantees greater robustness of the predictions. Moreover, we observe that in cases where there is (i) a smoother nominal prior, (ii) a smaller transport penalty in basis directions that induce roughness, (iii) a larger \( \delta \), or (iv) smaller nominal observational noise, the worst-case distributions induce sharper contrasts between the observed and unobserved locations along both the prior and posterior sample paths.

The remainder of this paper is organized as follows. We introduce our problem setup in Section 2. We present our main theoretical results in Section 3, illustrate the applicability of our general framework by highlighting several examples in Section 4, and present simple numerical experiments in Section 5. All proofs are deferred to the appendix.

## 2 Problem Statement

Let \( D \subset \mathbb{R}^d \), \( d \geq 1 \) be a compact set. We write \( C(D) \) to denote the space of real-valued continuous functions on \( D \), which is naturally endowed with the sup-norm \( \| \cdot \|_{C(D)} \). We denote by \( L^2(D) \) the space of real-valued square-integrable functions on \( D \). Since \( D \) is compact, we have \( C(D) \subseteq L^2(D) \).

We introduce a probability measure \( P_0 \) under which the so-called prior input process \( b_0 \) is a \( C(D) \)-valued centered Gaussian random field. Further, under the inclusion \( C(D) \hookrightarrow L^2(D) \) where \( \hookrightarrow \) denotes the inclusion map, the random field \( b_0 \) can be viewed as \( L^2(D) \)-valued. This random field generates a positive definite kernel, namely, \( K(x, x') = \mathbb{E}_{P_0}[b_0(x)b_0(x')] \) and thus an associated reproducing kernel Hilbert space (RKHS) which is obtained as the closure of functions of the form \( f(x) = \mathbb{E}_{P_0}[(a_1b_0(x_1) + \cdots + a_nb_0(x_n)b_0(x)] \). The closure can be taken relative to the norms \( \| \cdot \|_{C(D)} \) and \( \| \cdot \|_{L^2(D)} \); both limiting procedures coincide [36, Lemma 8.1]. By the spectral decomposition of the covariance operator of \( b_0 \) (i.e., \( K(\cdot, \cdot) \), [16, Example 2.6.15]), there exists a complete orthonormal system \( \{e_n\}_{n=1}^\infty \) of \( L^2(D) \) where \( e_n \in C(D) \), an i.i.d. sequence of standard univariate normal random variables \( \{g_n\}_{n=1}^\infty \), and a non-negative sequence of “eigenvalues” \( \{\kappa_n^2\}_{n=1}^\infty \) satisfying \( \sum_{n=1}^\infty \kappa_n^2 < \infty \), such that under \( P_0 \),

\[
b_0 = \sum_{n \geq 1} \kappa_n g_n e_n,
\]

where the convergence of the above infinite sum occurs in \( C(D) \), and thus also in \( L^2(D) \), almost surely. We impose a full-rank assumption on the prior \( b_0 \) in the following sense.

\footnote{For theory of Banach space-valued Gaussian random variables, we refer to [16, Chapter 2] and [36].}
Assumption 2.1 (Full rank). The closure of the RKHS generated by $b^0$ for the norm $\| \cdot \|_{C(D)}$ is equal to $C(D)$. Equivalently, $\kappa_n \neq 0$ for all $n \geq 1$.

Assumption 2.1 implies that the support of $b^0$ is not contained in a proper subspace of $C(D)$. This assumption is necessary to ensure that the worst-case distribution is unique in the proof of Theorems 3.1 and 3.2 below.

As an example, a general class of Gaussian smoothness priors can be constructed via the Laplace operator on $D$. Specifically, we will use the following class of Matérn processes in Sections 4 and 5, which provides natural prior distributions for $\alpha$-regular functions vanishing at the boundary $\partial D$.

Example 2.1 (Matérn prior [22, Equation (2)]). Suppose $D$ has a smooth boundary. The prior with a Matérn covariance function with parameters $\kappa \geq 0$ and $\alpha > \frac{d}{2}$ controlling the smoothness can be expressed as

$$b^0 = \sum_{n \geq 1} \left( \kappa^2 + \lambda_n \right)^{-\frac{d}{2}} g_n e_n,$$

where the eigenvalues $\lambda_n$ and eigenfunctions $e_n$ correspond to the Dirichlet-Laplacian operator on $D$ [34, Corollary 5.1.5]. The eigenvalues $\lambda_n$ satisfy Weyl’s law $\lambda_n = \Theta(n^{2/d})$ [35, Corollary 8.3.5] and the eigenfunctions $e_n \in C^\infty(\overline{D})$, $n \geq 1$, where $\overline{D}$ denotes the closure of $D$ and $C^\infty(\overline{D})$ is the space of infinitely smooth functions on $\overline{D}$.

We consider perturbations to the nominal prior $b^0$ by borrowing ideas from the field of distributionally robust optimization (DRO). We assume that the perturbations are supported in a space of continuous functions $H_w$ that is also a RKHS; in particular $H_w$ is also a Polish space, which is important to invoke key duality results to study the maximization in our DRO formulation. The useful feature of RKHS is that the point evaluation functionals are well-defined and continuous with respect to the Hilbert space norm. Specifically, we define the space

$$H_w = \left\{ f \in L^2(D) : \sum_{n \geq 1} w_n \langle f, e_n \rangle^2 < \infty \right\},$$

which is parameterized by a positive sequence $w = (w_n)_{n \geq 1}$. Notice that from this point, we abbreviate the inner product $\langle \cdot, \cdot \rangle_{L^2(D)}$ as $\langle \cdot, \cdot \rangle$. Typically, the Hilbert norm on $H_w$ is stronger than the usual $L^2(D)$ norm. More precisely, we impose the following assumption on $w$ and the basis $\{e_n\}_{n=1}^\infty$:

Assumption 2.2 (RKHS conditions). Assume that $\lim_{n \to \infty} w_n = \infty$ and $H_w$ is endowed with the inner product

$$\langle f, \tilde{f} \rangle_{H_w} = \sum_{n \geq 1} w_n \langle f, e_n \rangle \langle \tilde{f}, e_n \rangle \quad \forall f, \tilde{f} \in H_w.$$
Further, the space $H_w$ equipped with the Hilbert space norm $\| \cdot \|_{H_w}$ is a RKHS compactly embedded in $C(D)$.

Under Assumption 2.2, $H_w$ is a separable Hilbert space such that point evaluation functionals are well-defined and continuous. Note that the sequence $w$ controls the roughness (or equivalently the smoothness) of functions in $H_w$. Throughout the rest of the paper we will fix a given sequence $w$ satisfying Assumption 2.2. The norm $\| \cdot \|_{H_w}$ will be used to define our adversarial perturbations. The next example, which is a continuation of Example 2.1, provides intuition about the interpretation of $w$ in terms of roughness.

**Example 2.2 (RKHS space).** Let the eigenvalues $\lambda_n$ and eigenfunctions $e_n$ correspond to the Dirichlet-Laplacian operator on $D$. Consider $w_n = \Theta(\lambda_n^{\beta/2})$. Then $\beta$ controls the roughness of functions in $H_w$. Note that the “spectrally defined” spaces $H_w$ are subspaces of the classical Sobolev spaces on $D$. Thus for any $\beta > \frac{d}{2}$, by the Sobolev embedding theorem [24, Proposition 4.1.3], we can identify $f \in H_w$ with its continuous version. Under this identification $H_w$ is a RKHS in $C(D)$.

Now suppose that we have a linear “forward” operator $T$ that maps sample paths of the prior input process $b^0$ to sample paths of another process $u$, which also takes values in $C(D)$. We make the following assumptions on this operator.

**Assumption 2.3 (Operator).** We assume the following:

(i) The forward map $T : C(D) \to C(D)$ is linear and bounded (with operator norm $C_T > 0$).

(ii) There exists a positive sequence $\tilde{w} = \{\tilde{w}_n\}_{n=1}^{\infty}$ and a corresponding space $H_{\tilde{w}}$ as in (3), with Hilbert space norm $\| \cdot \|_{H_{\tilde{w}}}$, which constitutes a RKHS continuously embedded in $C(D)$ such that for some positive constant $C_{\tilde{w}}$,

$$
\|T(f)\|_{H_{\tilde{w}}} \leq C_{\tilde{w}} \|f\|_{H_{\tilde{w}}}, \quad \forall f \in H_{\tilde{w}}.
$$

In other words, $T$ is bounded when restricted to $H_{\tilde{w}}$.

The forward operator $T$ defines our data-generating process. In particular, let $x_i \in D$, $i = 1, \ldots, m$ be the design points. Also under $P_0$, let $\epsilon^0 = (\epsilon^0_1, \ldots, \epsilon^0_m)$ be a vector of independent $\mathcal{N}(0, \sigma^2)$ errors. Then we observe single path of $u$, with noise, at the design points, i.e.,

$$
Y_i = u^0(x_i) + \epsilon^0_i, \quad i = 1, \ldots, m,
$$

where $u^0(x_i) = T(b^0)(x_i)$, $i = 1, \ldots, m$ are point evaluations of a single sample path. We further assume that both $b^0$ and $\epsilon^0$ are independent under $P_0$. Consequently, under $P_0$,

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2For positive sequences $\{a_n\}, \{b_n\}$, the notation $a_n = \Theta(b_n)$ means that $1/c_0 \leq a_n/b_n \leq c_0$, for some $c_0 \in (0, \infty)$. 

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the pair \((b_0, e_0)\) constitutes a Gaussian random variable on the product space \(C(D) \times \mathbb{R}^m\) (which is Banach with the product norm).

We will see examples in Section 4 where Assumption 2.3 on the forward operator is satisfied; these include Gaussian process regression (where \(T = \text{Id}\)) and several canonical linear inverse problems. Assumption 2.3 entails certain compatibility of the forward operator with the prior basis \(\{e_n\}_{n=1}^\infty\), which is similar to the assumption of “norm equivalence on regularity scales” in the literature on linear Bayesian inverse problems \([17, 2]\). We note that other assumptions in the literature exist, e.g., the “band-limited” assumption in \([27]\). In our framework, we will consider Wasserstein perturbations to the prior \(P_0\), which encompass a much richer collection of prior families than typically considered in the literature.

2.1 The nominal estimation problem

Let \(M\) denote the space of measurable maps from \(\mathbb{R}^m\) (data space) to \(C(D)\) (parameter space) and let \(P\) denote the space of (Borel) probability measures on \(C(D) \times \mathbb{R}^m\). The classical Bayes risk minimization for \(L^2(D)\) loss is

\[
\min_{\phi \in M} \mathbb{E}_{P_0} \left[ \|u_0 - \phi(Y_1, \ldots, Y_m)\|_{L^2(D)}^2 \right],
\]

where \(\phi(Y_1, \ldots, Y_m)\) is the predictor for \(u_0\) given observations \((Y_1, \ldots, Y_m)\). We regard the problem as the nominal estimation problem since the Bayes risk is evaluated under the nominal measure \(P_0\). The solution of the nominal problem is the posterior mean (or conditional expectation), i.e.,

\[
\phi_0(Y_1, \ldots, Y_m)(x) = \mathbb{E}_{P_0} \left[ u_0(x) | Y_1, \ldots, Y_m \right].
\]

This follows by noting that the \(L^2(D)\)-norm is a Lebesgue integral and using Fubini’s theorem. Since we assume that the nominal distribution \(P_0\) is Gaussian, this estimator corresponds to the linear prediction rule,

\[
\mathbb{E}_{P_0} \left[ u_0(x) | Y_1, \ldots, Y_m \right] = (k(x, x_1), \ldots, k(x, x_m)) \cdot (K)^{-1} \cdot (Y_1, \ldots, Y_m)^\top,
\]

where \(k(x, x_i) = \mathbb{E}_{P_0}[u_0(x)Y_i]\), \(K_{ij} = (\mathbb{E}_{P_0}[Y_i Y_j])\), and \(K \in S^m_{++}\), where \(S^m_{++}\) denotes the set of strictly positive definite matrices.

In the introduction, we wrote in \([1]\) an analogous estimation problem for \(b_0\), which we shall revisit below. For non-identity \(T\), \([1]\) corresponds to solving a linear inverse problem while \([4]\) is regression (e.g., imputing the rest of \(u_0\) given noisy pointwise observations).

2.2 Distributionally robust optimization formulation

Instead of considering the nominal measure \(P_0\) on the prior and noise distributions, we postulate a min-max game where an adversary chooses a measure \(P\) in opposition of the
decision-maker’s choice of estimator. In particular, for some forward map $T$ describing the relationship between the parameter $b$ and the regression function $u = T(b)$, we assume that the observations $Y_1, \ldots, Y_m$ arise as
\[
\begin{cases}
(b, \epsilon_1, \ldots, \epsilon_m) \sim P, \\
Y_1 = u(x_1) + \epsilon_1, \ldots, Y_m = u(x_m) + \epsilon_m,
\end{cases}
\tag{5}
\]
where $u(x_1), \ldots, u(x_m)$ are point evaluations of a single sample path. Instead of the nominal Bayes risk, we consider a ‘worst-case Bayes risk’ with respect to all possible mis-specification on both $b$ and $\epsilon$, i.e., the whole data-generating process. Our goal is to minimize the worst-case Bayes risk by solving
\[
\inf_{\phi \in \mathcal{M}} \sup_{P \in \mathcal{P}, \mathcal{W}(P, P_0) \leq \delta} \mathbb{E}_P \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right],
\tag{6}
\]
where nature’s admissible choice of $P$ is constrained by the Wasserstein distance $\mathcal{W}(P, P_0)$ relative to the nominal measure $P_0$. We will also consider the analogous robust formulation for estimating $b$ itself, as written in [2]; we revisit this formulation specifically in Section 3.3.

The Wasserstein distance $\mathcal{W}$ above is constructed as follows.

**Definition 2.1** (Optimal transport cost). The optimal transport cost between two probability measures on $C(D) \times \mathbb{R}^m$ is defined as
\[
D_c(P, P_0) = \inf \{ \mathbb{E}_\pi[c((b, \epsilon), (b^0, \epsilon^0))] : \pi((b, \epsilon)) = P, \pi((b^0, \epsilon^0)) = P_0 \},
\tag{7}
\]
where the infimum is taken over all couplings $\pi$ between $(b, \epsilon)$ and $(b^0, \epsilon^0)$ with marginals $P$ and $P_0$, and $c$ is some ground cost on $C(D) \times \mathbb{R}^m$.

The existence of an optimal coupling (i.e., an optimal solution to problem (7)) is guaranteed whenever $c$ is non-negative and lower semi-continuous with respect to the product norm on the Polish space $(C(D) \times \mathbb{R}^m)^2$; see e.g. [37, Theorem 4.1]. In this paper, we use the ground cost function $c$ defined as
\[
c((b, \epsilon), (b^0, \epsilon^0)) = \| \epsilon - \epsilon^0 \|^2_2 + \| b - b^0 \|^2_{L^2_w} = \sum_{i=1}^m (\epsilon_i - \epsilon_i^0)^2 + \sum_{n \geq 1} \left( \langle b, e_n \rangle - \langle b^0, e_n \rangle \right)^2 w_n.
\]

To see that $c$ is lower semi-continuous, note that if $\| b_k - b_\infty \|_{C(D)} \to 0$ and $\| \tilde{b}_k - \tilde{b}_\infty \|_{C(D)} \to 0$ as $k \to \infty$, then
\[
\liminf_{k \to \infty} \left( \langle b_k, e_n \rangle - \langle \tilde{b}_k, e_n \rangle \right)^2 w_n \geq \left( \langle b_\infty, e_n \rangle - \langle \tilde{b}_\infty, e_n \rangle \right)^2 w_n
\]
for each $n$ since $e_n \in C(D)$. Thus
\[
\liminf_{k \to \infty} \sum_{n \geq 1} \left( \langle b_k, e_n \rangle - \langle \tilde{b}_k, e_n \rangle \right)^2 w_n \geq \sum_{n \geq 1} \left( \langle b_\infty, e_n \rangle - \langle \tilde{b}_\infty, e_n \rangle \right)^2 w_n.
\]
With this choice of the ground cost $c$, the optimal coupling between $P$ and $P_0$ exists for any $P$ and $P_0$. Note that $D_c$ is not a distance because it does not satisfy the triangle inequality, but its square root $W := \sqrt{D_c}$ is a Wasserstein-type distance on its domain of finiteness $\{P \in \mathcal{P} : D_c(P, P_0) < \infty\}$ [37, Definition 6.1].

It is important to stress that our $W$ depends on the specification of the function class $\mathcal{H}_w$, or equivalently on the Hilbert space norm $\| \cdot \|_{\mathcal{H}_w}$. This dependence provides a convenient tool to control features such as the amount of roughness or smoothness that the adversary is allowed to inject in the sample path of the process $b$ (and hence of $u$). Intuitively speaking, the sequence $w$ puts different penalties on the mass transportation of different “modes” of the spectral decomposition of the sample path of $b$. For example, if the sequence $w$ increases to infinity slowly, then the adversary is under-penalized for moving mass corresponding to the higher “modes,” resulting in rougher sample paths of $b$. The modeling of the behavior of the adversary thus conveniently reduces to the specification of the Hilbert norm $\| \cdot \|_{\mathcal{H}_w}$.

We impose a final compatibility assumption between the operator $T$ and the adversarial cost introduced.

**Assumption 2.4** (Operator and adversarial cost). Suppose that we can select $\tilde{w}$ in Assumption 2.3 such that $\tilde{w}_n = o(w_n)$ as $n \to \infty$.

Intuitively, Assumption 2.4 simply says that the operator is bounded even if the adversarial perturbations are made to be slightly rougher than the adversarial choice. This assumption, we believe, is purely technical. The natural condition to impose is that the operator is bounded only on the chosen adversarial space. Our results hold under this more natural (and weaker) assumption in the case of standard Gaussian process regression, namely when $T$ equals the identity map.

**Remark 2.1.** Having introduced the setup of our framework, a few comments are in order.

(i) It is natural to consider random elements on a general Banach space $\mathcal{B}$ other than $C(\mathcal{D})$, e.g., by embedding the Banach space $\mathcal{B}$ in its second dual $\mathcal{B}^{**}$ and identify a Borel measurable random element $b$ in $\mathcal{B}$ with the stochastic process $(b^*(b) : b^* \in \mathcal{B}^*)$, but at the expense of technicality, see a discussion in [36, Section 2.3]. We choose $C(\mathcal{D})$ to mainly illustrate our conceptual contribution of a distributionally robust formulation of nonparametric regression and inverse problems.

(ii) The $L^2(\mathcal{D})$ norm in the objective function of the formulation can potentially be replaced by another member in the hierarchy of the Hilbert space norms. However, the latter norm lacks the Lebesgue integral representation, especially for those with fractional power [34, Section 4.1], and we leave the extension to a future work.

(iii) It is tempting to replace the Hilbert space norm with the $L^2(\mathcal{D})$ norm in the definition of the ground cost function $c$. However, point evaluations are not continuous under
the $L^2(D)$ norm. Our proofs for the main results rely crucially on the continuity of point evaluations, and thus we resort to the RKHS in Assumption 2.3.

3 Main Results

3.1 Strong duality

Our first main result is a minimax theorem, which states that one may interchange the infimum and supremum operators in the regression problem (6).

**Theorem 3.1** (Strong duality for the regression problem). Suppose that Assumptions 2.1–2.4 hold. For any $\delta > 0$, the strong duality holds:

$$
\inf_{\phi \in \mathcal{M}} \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \mathbb{E}_P \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right] = \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \inf_{\phi \in \mathcal{M}} \mathbb{E}_P \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right].
$$

(8)

The idea of the proof to Theorem 3.1 is to first show a strong duality result for a sequence of finite-dimensional approximations. In particular, define span$\{e_n\}_{n=1}^N$ as the (closed) linear subspace of $C(D)$ spanned by the basis vectors $(e_n : 1 \leq n \leq N)$. We consider truncating $P$ (resp. $P_0$) into the space span$\{e_n\}_{n=1}^N \times \mathbb{R}^m$, and denote the induced measure as $Q(N)$ (resp. $Q_0(N)$). The truncation is through the coordinate projections after expanding functions in the $L^2(D)$ basis $\{e_n\}_{n=1}^\infty$. Since the coordinate projections are bounded linear mappings, $Q_0(N)$ is centered Gaussian. Notice that the space span$\{e_n\}_{n=1}^N \times \mathbb{R}^m$ is isomorphic to $\mathbb{R}^{N+m}$, thus we view the truncated measures $Q(N)$ and $Q_0(N)$ as finite-dimensional measures on $\mathbb{R}^{N+m}$.

For convenience, denote

$$
\text{Obj}(\phi, P) = \mathbb{E}_P \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right],
$$

and by a slight abuse of notation we denote $\text{Obj}(\phi, Q(N))$ for the truncated measure. In the proof we construct the finite-dimensional approximations, and the related strong duality reads

$$
\min_{\phi \in \mathcal{M}} \max_{Q(N) : W_N(Q(N), Q_0(N)) \leq \delta} \text{Obj}(\phi, Q(N)) = \max_{Q(N) : W_N(Q(N), Q_0(N)) \leq \delta} \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, Q(N)),
$$

(9)

where $W^2_N$ is the induced optimal transport cost on $\mathbb{R}^{N+m}$

$$
W^2_N(Q(N), Q_0(N)) = \min_{\pi} \left\{ \mathbb{E}_{\pi}[c_N(r, s) : \pi_r = Q(N), \pi_s = Q_0(N)] \right\}.
$$
Here $\pi_r$ and $\pi_s$ are projections onto the first and second component of the coupling $\pi$. In the definition of $W_N^2$, $c_N$ is the induced cost function on $\mathbb{R}^{N+m}$ with

$$c_N(r,s) = \sum_{n=1}^{N} (r_n - s_n)^2 w_n + \sum_{j=1}^{m} (r_{N+j} - s_{N+j})^2 \quad \text{for any } r, s \in \mathbb{R}^{N+m}.$$ 

We note that in (9), the minimizer in the $\phi$ variable and the maximizer in the $Q(N)$ variable exist, which justifies the minimization and the maximization operators. Denote by $\phi^{\star}_N$ (resp. $Q^{\star}_N$) the (unique) solution to the outer optimization problem in the left-hand (resp. right-hand) side of (9). Then $(\phi^{\star}_N, Q^{\star}_N)$ is the (unique) pair of Nash equilibrium for problem (9) in the sense that

$$\text{Obj}(\phi^{\star}_N, Q^{\star}_N) = \min_{\phi \in M} \text{Obj}(\phi, Q^{\star}_N) = \max_{Q(N) : W_N(Q(N), Q_0(N)) \leq \delta} \text{Obj}(\phi^{\star}_N, Q(N)).$$

The structural properties of the optimal solutions reveal that $Q^{\star}_N$ is a centered Gaussian distribution, and $\phi^{\star}_N$ is a linear prediction rule. Namely, for any $x \in D$,

$$\phi^{\star}_N(Y_1, \ldots, Y_m)(x) = \mathbb{E}_{Q_N}[u(x)|Y_1, \ldots, Y_m] = (k^{(N)}_e(x,x_1), \ldots, k^{(N)}_e(x,x_m)) \cdot (K^{(N)}_e)^{-1} \cdot (Y_1, \ldots, Y_m)^\top,$$

where $k^{(N)}_e(x,x_i) = \mathbb{E}_{Q_N}[u(x)Y_i]$, and $K^{(N)}_e = \left(\mathbb{E}_{Q_N}[Y_iY_j]\right)_{ij} \in \mathbb{S}^{m}_{++}$ is invertible. Similar finite-dimensional duality results have been established in [25, 28], but with a different definition of the Wasserstein distance and the ambiguity set. The rest of the proof then argues that the error of approximations is negligible as the dimension $N$ grows to infinity.

In particular, one intermediate result we rely on in Section 5 is the following.

**Proposition 3.1 (Approximation of objective values).** Let $\phi^{\star}_N$ be the (unique) solution to the min-max problem in (9), and $Q^{\star}_N$ be the (unique) solution to the max-min problem in (9). We have

$$\text{Obj}(\phi^{\star}_N, Q^{\star}_N) = \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \text{Obj}(\phi^{\star}_N, P) + o(1) = \inf_{\phi \in \mathcal{M}} \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \text{Obj}(\phi, P) + o(1),$$

asymptotically as the number of basis vectors in the approximation tends to infinity, i.e., as $N \to \infty$.

### 3.2 Existence, uniqueness, and construction of the Nash equilibrium

In this part we show that (8) admits a unique pair of Nash equilibrium under certain conditions. Recall the Nash equilibrium $(\phi^{\star}_N, Q^{\star}_N)$ corresponding to the finite dimensional
approximately in the last section. We now add the tail of $P_0$ to $Q^*_N$, namely, we denote $P^*_N \in \mathcal{P}$ as the measure under which the two random elements

$$\{\{b, e_n\}_{n=1}^N\} \text{ and } \{\{b, e_n\}_{n=N+1}^\infty\}$$

are independent. Moreover, we have that

$$P^*_N \approx P_0$$

in the last section. We now add the tail of $P^*_N$, $N \geq 1$ by a compactness argument.

**Proposition 3.2** (Compactness of the ambiguity set). Under the conditions of Theorem [3.1], for every sequence $P_N \in \mathcal{P}, N \geq 1$ that satisfies $W(P_N, P_0) \leq \delta$, there exists a weakly convergent subsequence $P_{N_l}', \ldots, P_{N_m}'$, such that the limit $P_\infty \in \mathcal{P}$ also satisfies $W(P_\infty, P_0) \leq \delta$.

By Proposition 3.2, we find a weakly convergent subsequence of $P^*_N$, denoted as $P^*_{N_l}'$, $l \geq 1$, with a limit $P^*_\infty$ that is feasible. The subsequence $P^*_{N_l}'$ is centered Gaussian, thus the limit $P^*_\infty$ is also centered Gaussian. To see this, consider any bounded linear functional $F : C(\mathcal{D}) \times \mathbb{R}^m \rightarrow \mathbb{R}$, and construct the Skorohod representations $Z_{N_l} \sim P^*_{N_l}'$ and $Z_{\infty} \sim P^*_\infty$, where $Z_{N_l}$ converges to $Z_{\infty}$ almost surely on the common probability space. It follows that $F(Z_{N_l})$ converges to $F(Z_{\infty})$ almost surely, and we note that the limit of centered univariate Gaussians must also be centered univariate Gaussian.

Define the matrix $K_\epsilon = (E_{P^*_\infty}[Y_{ij}])_{i,j} \in \mathbb{S}^m_+$. Under the condition that $K_\epsilon$ is invertible, the solution $\phi^*_\infty$ to $\min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^*_\infty)$ is well-defined as

$$\phi^*_\infty(Y_1, \ldots, Y_m)(x) = E_{P^*_\infty}[u(x) | Y_1, \ldots, Y_m]$$

$$= (k_\epsilon(x, x_1), \ldots, k_\epsilon(x, x_m)) \cdot (K_\epsilon)^{-1} \cdot (Y_1, \ldots, Y_m)^\top,$$

where $k_\epsilon(x, x_i) = E_{P^*_\infty}[u(x)Y_i]$. The main result of this section is the following theorem.

**Theorem 3.2** (Nash equilibrium). Suppose that the conditions of Theorem [3.1] hold. Let $P^*_\infty$ denote the limit of a weakly convergent subsequence of $P^*_N$, and assume that $K_\epsilon$ is invertible under $P^*_\infty$. Then, for $\phi^*_\infty$ given by (11), the pair $(\phi^*_\infty, P^*_\infty)$ forms a Nash equilibrium to problem (8), i.e.,

$$\text{Obj}(\phi^*_\infty, P^*_\infty) = \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^*_\infty) = \max_{P \in \mathcal{P} : W(P, P_0) \leq \delta} \text{Obj}(\phi^*_\infty, P).$$

Thus $(\phi^*_\infty, P^*_\infty)$ represents a pair of equilibrium strategies where neither the decision-maker nor the adversary (the two players of the game) benefits from changing their own strategy. Moreover, the pair $(\phi^*_\infty, P^*_\infty)$ is unique, with components respectively given by the pointwise limit

$$\lim_{N \to \infty} \phi^*_N(Y_1, \ldots, Y_m)(x) = \phi^*_\infty(Y_1, \ldots, Y_m)(x), \quad \forall Y_1, \ldots, Y_m \in \mathbb{R}, \quad x \in \mathcal{D},$$

and the weak limit $P^*_N \Rightarrow P^*_\infty$ as $N \to \infty$. 


One important consequence of Theorem 3.2 is that the worst-case distribution involves a modified Gaussian process with potentially rougher paths than the prior. Hence the robustified decision, as the conditional mean of the worst-case distribution, remains affine in the observations and therefore is tractable. The convergence statement in Theorem 3.2 readily gives rise to an algorithm for computing the associated Nash equilibrium.

The result of Theorem 3.2 requires that $K_\epsilon$ is invertible for the limit of some weakly convergent subsequence of $P_N^\star$. Fortunately, due to the following proposition, it is not difficult to check whether this condition holds in practice.

**Proposition 3.3.** Either one (and only one) of the following cases occurs.

1. there exists a weakly convergent subsequence of $P_N^\star$, with the limit denoted by $P_\infty^\star$, such that the matrix $K_\epsilon$ is invertible under $P_\infty^\star$, or

2. the sequence of determinants $\det(K_\epsilon^{(N)}) \to 0$ as $N \to \infty$.

To conclude this section, we provide a sufficient condition to ensure that the first case of Proposition 3.3 occurs.

**Lemma 3.3 (Invertibility).** There exists a strictly positive constant $\delta_0$ that depends on $(T,m,(x_i)_i,\mathcal{H}_w,\mathcal{H}_{\tilde{w}},\sigma^2)$ such that for any $\delta < \delta_0$ and $P$ satisfying $W(P,P_0) \leq \delta$, the matrix $(\mathbb{E}_P[Y_i Y_j])_{ij}$ is invertible.

### 3.3 Strong duality for the inverse problem

Alternatively, we propose a distributionally robust formulation for the inverse problem, where our primary interest lies in recovering the unknown input $b$. Under the observation system (5), the goal of the decision-maker is to seek for a nonparametric predictor $\phi_b \in \mathcal{M}$ that minimizes the worst-case objective

\[
\inf_{\phi_b \in \mathcal{M}} \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \mathbb{E}_P \left[ \|b - \phi_b(Y_1, \ldots, Y_m)\|_{L^2(D)}^2 \right], \tag{12}
\]

where nature’s admissible choice of $P$ is constrained by the Wasserstein distance $W(P,P_0)$ constructed from (7). We state the strong duality of (12).

**Theorem 3.4 (Strong duality for the inverse problem).** Suppose that Assumptions 2.1–2.4 hold. For any $\delta > 0$,

\[
\inf_{\phi_b \in \mathcal{M}} \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \mathbb{E}_P \left[ \|b - \phi_b(Y_1, \ldots, Y_m)\|_{L^2(D)}^2 \right] = \sup_{P \in \mathcal{P}, W(P,P_0) \leq \delta} \inf_{\phi_b \in \mathcal{M}} \mathbb{E}_P \left[ \|b - \phi_b(Y_1, \ldots, Y_m)\|_{L^2(D)}^2 \right]. \tag{13}
\]
The proof of Theorem 3.4 works verbatim as that of Theorem 3.1. Though strong duality holds for both the regression and the inverse problems under our formulations, we note that for ill-posed inverse problems in the Bayesian nonparametrics literature, the minimax rate for estimating $b$ is slower than the minimax rate for estimating $u$ \cite{12,8,9,19}.

As to the Nash equilibrium associated with (13), it is not hard to see, after examining the proof of Theorem 3.2, that we can develop the same theory verbatim to that of Section 3.2. For ease of exposition, we suppress the details here.

4 Some Examples

In this section we give several examples that illustrate the applicability of our general framework. We restrict our attention to Matérn process priors and the Sobolev-type space of perturbations given by Examples 2.1 and 2.2 respectively. We assume the relation $\kappa_n = \lambda_n^{-\alpha/2}$ (so that $\kappa = 0$ in Example 2.1) and $w_n = \lambda_n^\beta$, where $\alpha > d/2$ and $\beta > d/2$.

Example 4.1 (Gaussian process regression). By choosing $T$ as the identity operator, we recover Gaussian process regression. Assumptions 2.3–2.4 are satisfied for $\tilde{w}_n = \lambda_n^\tilde{\beta}$ and any $d/2 < \tilde{\beta} < \beta$. If $D$ is the one-dimensional interval $[0, 1]$, the eigenvalues are $\lambda_n = n^2 \pi^2$, and the eigenfunctions are

$$e_n(x) = \sqrt{2} \sin(n\pi x) \quad \forall x \in [0, 1].$$

Example 4.2 (Laplace equation). The Laplace equation with a homogeneous Dirichlet boundary condition is

$$\begin{cases}
\Delta u(x) = b(x) & \forall x \in D^o, \\
u(x) = 0 & \forall x \in \partial D,
\end{cases}$$

where $D^o$ is the interior of $D$, while $\partial D$ denotes its boundary. We have that the forward map $T$ is the inverse-Laplacian operator, thus

$$T(f) = \sum_{n \geq 1} -\lambda_n^{-1}(f, e_n)e_n.$$ 

It is straightforward to see that Assumptions 2.3, 2.4 are satisfied for $\tilde{w}_n = \lambda_n^{\tilde{\beta}}$ and any $d/2 < \tilde{\beta} < \beta$.

Example 4.3 (Heat equation). The one-dimensional homogeneous heat equation without source is

$$\begin{cases}
u_t = \nu_{xx} & 0 < x < 1, \\
u(x, 0) = b(x) & 0 < x < 1, \\
u(0, t) = \nu(1, t) = 0 & t \geq 0,
\end{cases}$$

15
where \( u(\cdot, t) \) is the temperature profile at time \( t \), and \( b \) is the initial condition. By separation of variables, the solution to the heat equation is

\[
    u(x, t) = \sum_{n \geq 1} e^{-n^2 \pi^2 t} \langle b, e_n \rangle e_n.
\]

Therefore, the (time-dependent) forward map \( T \) satisfies, for any \( t \geq 0 \),

\[
    T(f) = \sum_{n \geq 1} e^{-n^2 \pi^2 t} \langle f, e_n \rangle e_n.
\]

Assumptions 2.3–2.4 are satisfied for \( \tilde{w}_n = \lambda_n^{\beta} \) and any \( \frac{d}{2} < \tilde{\beta} < \beta \).

**Example 4.4** (Radon transform in the plane). The Radon transform of a function \( f \) is the function

\[
    T(f)(s, \omega) = \int_{-\infty}^{\infty} f(s\omega + t\omega^\perp)dt, \quad s \in \mathbb{R}, \ \omega \in S^1,
\]

where \( S^1 \) is the unit circle and \( \omega^\perp \) is the vector in \( S^1 \) obtained by rotating \( \omega \) counterclockwise by 90°. Recall we consider \( f \) to be supported in a compact domain \( D \subset \mathbb{R}^2 \), and thus \( T(f) \) vanishes outside a compact subset of \( \mathbb{R} \times S^1 \). It is straightforward to see that \( T : C(D) \to C(\mathbb{R} \times S^1) \) is linear and bounded, where we allow a slight modification of our framework since \( T \) takes value in a different space from its domain of definition. By [24, Theorems II.5.1 and II.5.2], the Radon transform has the Sobolev estimate:

\[
    \|T(f)\|_{H^{\tilde{\beta}}(\mathbb{R} \times S^1)} \leq C_{\tilde{w}} \|f\|_{H_{\tilde{w}}}, \quad \forall f \in H_{\tilde{w}},
\]

for \( \tilde{w}_n = \lambda_n^{\beta} \) and any \( 1 = \frac{d}{2} < \tilde{\beta} < \beta \), where \( H^{\tilde{\beta}}(\mathbb{R} \times S^1) \) is the usual order-\( \tilde{\beta} \) Sobolev space. Identifying \( S^1 \) with \([0, 2\pi]\), and by the Sobolev embedding theorem [34, Proposition 4.1.3], we see that point evaluations in \( H^{\tilde{\beta}}(\mathbb{R} \times S^1) \) are continuous. Our theory in Section 3 applies with this slight modification of Assumptions 2.3.2.4 after inspecting the proofs.

## 5 Numerical Experiments

Our focus in this paper is formulating a min-max framework for regression and inverse problems in an infinite-dimensional setting, and elucidating key theoretical properties of this formulation. We now present some numerical experiments that offer further insights into the properties of the Nash equilibrium. In particular, we compute the Nash equilibrium \( (\phi_N^*, Q_N^*) \) of a finite-dimensional approximation of the robust estimation problem (see definitions in Section 3) with \( N = 200 \), by an adaptation of the Frank-Wolfe algorithm in [28]. Under the conditions of Theorem 3.2, the use of the finite-dimensional Nash equilibrium is justified. When the condition fails, Proposition 3.1 still guarantees that the objective
values of the finite-dimensional games converge to those of the infinite-dimensional games. We illustrate our results for Gaussian process regression on the unit interval $D = [0,1]$, as described in Example 4.1. Throughout this section we set $\kappa_n = \lambda_n^{-\alpha/2}$ and $w_n = \lambda_n^\beta$. Recall that $(\kappa_n)_{n \geq 1}$, and hence $\alpha$, control the smoothness of the nominal prior; while $(w_n)_{n \geq 1}$, and hence $\beta$, control the roughness of the adversarial perturbations to the prior via the $\|\cdot\|_{\mathcal{H}_w}$ component of the transport cost.

First we fix a set of baseline parameters: $\alpha = 2$ and $\beta = 0.51$; $\delta^2 = 0.1$ (size of the Wasserstein ball); and $\sigma = 0.1$ (observational noise magnitude). We choose $m = 10$ design points $(x_i)_{i=1}^{10}$ equispaced on either the $(0,1)$ or $(0,0.5)$ intervals, excluding the endpoints. More specifically, we choose $x_i = i/11$ and $x_i = i/22$ respectively. Below we visualize the prior and posterior covariances of $b$ under the nominal and worst-case measures $Q_0^{(N)}$ and $Q_N^*$; i.e., $\text{Cov}_P[b]$ and $\text{Cov}_P[b|y_1, \ldots, y_m]$ for $P \in \{Q_0^{(N)}, Q_N^*\}$. Since both the nominal and the worst-case measures are Gaussian, the posterior covariances do not depend on the realization of the data.

We first visualize the four correlation functions corresponding to these covariances, for our two designs, in Figures 1 and 2. The geometry of each design is evident in the worst-case measures. Compared to the nominal measures, we observe that there are “ripples” in the worst-case measures corresponding to reductions of correlation between the observed locations. Next, in Figures 3 and 4, we plot marginal intervals (at each $x$) containing 95% of the nominal and the worst-case sample paths. Data to obtain the two posteriors shown here were draws from the nominal prior measure. In particular, we used the vector of observations

$$(-0.17, -0.09, 0.02, 0.04, 0.12, 0.05, -0.03, 0.03, -0.28, -0.15)$$

for the $(0,1)$ design and

$$(0.03, -0.05, 0.08, -0.08, 0.15, 0.12, -0.25, -0.24, 0.16, 0.02)$$

for the $(0,0.5)$ design. Comparing to the nominal prior measures, we observe that the worst-case prior measures have roughly the same overall variance magnitude, but a sharper contrast between the observed and unobserved locations, especially for the $(0,1)$-equispaced designs. On the other hand, comparing to the nominal posterior measures, we observe that the worst-case posterior measures have significantly higher marginal variances in regions away from the observed locations, while the variance increase moderately in regions surrounding the observations. The worst cases are thus perturbed so as to induce greater uncertainty in regions where information is limited; intuitively, this guarantees greater robustness of the estimates.

We next vary the baseline parameters to see the effect of the worst-case perturbations on (prior and posterior) sample paths of $b$, compared to sample paths of $b$ under the nominal measures. We focus on the $(0,1)$-equispaced design. For each parameter setting, we draw and visualize five independent sample paths, to gauge their qualitative behavior.
The posterior sample paths are conditioned on the same observation values as before. As another way of quantifying the impact of the worst-case perturbation, we compute the distance between the prior and posterior covariance matrices on $S^N_{++}$, where these matrices are induced by either the nominal or the worst-case measure. The distance we employ is the natural geodesic distance on the manifold of symmetric positive-definite matrices, also known as the Förstner distance [13] and (up to a constant) Rao’s distance [3, 26]. This distance is invariant under affine transformations and under inversion, and has been used extensively to compare covariance matrices in previous work [13, 32, 31]. With the remaining parameters fixed to the base case, we explore the following parameter variations.

1. Prior smoothness: choose $\alpha \in \{0.51, 2, 4\}$. Results are shown in Figures 5–7; note that we include the baseline value $\alpha = 2$ for comparison.
2. Adversarial perturbation smoothness: choose $\beta \in \{0.7, 1\}$. Results are shown in Figure 8. Note that the nominal prior and posterior are the same as in the baseline setting.

3. Size of the Wasserstein ambiguity set: choose $\delta^2 \in \{0.01, 1\}$. Results are shown in Figure 9. Note that the nominal prior and posterior are the same as in the baseline setting.

4. Magnitude of the observation noise: choose $\sigma \in \{0.01, 1\}$. Results are shown in Figures 10 and 11.

The corresponding nominal and worst-case prior-to-posterior distances are reported Table 1. Combining these qualitative and quantitative results, we observe that in cases where there is: a larger $\alpha$ (i.e., a smoother prior); a smaller $\beta$ (i.e., smaller penalty on
modes that induce roughness); a larger $\delta$ (i.e., wider range of admissible perturbations); or a smaller $\sigma$ (i.e., smaller observation noise), the worst-case distributions induce sharper contrasts between the observed and unobserved locations in both the prior and posterior sample paths.

$$
\begin{array}{cccccccc}
\alpha = 0.51 & 4 & \beta = 0.7 & 1 & \delta^2 = 0.01 & 1 & \sigma = 0.01 & 1 \\
2.56 & 2.56 & 2.56 & 2.56 & 2.56 & 2.56 & 8.92 & 0.11 \\
12.82 & 16.15 & 5.33 & 8.97 & 2.13 & 9.88 & 10.90 & 19.74 & 3.64 \\
\end{array}
$$

Table 1: Natural distance between the prior and posterior covariance matrices under different problem settings, for 10 design points equispaced on (0, 1).
Figure 4: 95% intervals of sample paths with 10 design points equispaced on (0, 0.5).

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Figure 5: Sample paths with $\alpha = 0.51$ and 10 designs equispaced in $(0, 1)$.

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6 Appendix

6.1 Proof of Theorem 3.1

Proof of the strong duality. We start with a few definitions used in the proof. Recall that $\mathcal{M} = \{\phi : \mathbb{R}^m \to C(\mathcal{D}), \phi \text{ is measurable}\}$ is the set of estimators for $u$.

Definition 6.1 (Affine predictor). For $\phi(Y_1, \ldots, Y_m)$ a mapping from $\mathbb{R}^m$ (data space) to $C(\mathcal{D})$ (parameter space), we say that $\phi$ is affine if it is of the form

$$\phi(Y_1, \ldots, Y_m) = \alpha_0 + \sum_{j=1}^{m} \alpha_j Y_j,$$

for some functions $\alpha_j \in C(\mathcal{D})$, $0 \leq j \leq m$. We write $\mathcal{M}_{\text{aff}} = \{\phi : \mathbb{R}^m \to C(\mathcal{D}), \phi \text{ is affine}\} \subset \mathcal{M}$.

Let $\text{span}\{e_n\}_{n=1}^N$ and $\text{span}\{T(e_n)\}_{n=1}^N$ denote the closed subspaces of $C(\mathcal{D})$ spanned by the first $N$ basis functions from Assumption 2.1, and by the action of $T$ on these basis, respectively. For affine $\phi$, we say that $\text{coef}(\phi) \in \text{span}\{T(e_n)\}_{n=1}^N$ if for all $0 \leq j \leq m$, $\alpha_j \in \text{span}\{T(e_n)\}_{n=1}^N$, and we denote the set of such estimators by $\mathcal{M}_{\text{aff},N} = \{\phi \in \mathcal{M}_{\text{aff}} : \text{coef}(\phi) \in \text{span}\{T(e_n)\}_{n=1}^N\}$.

For convenience, we write

$$\text{Obj}(\phi, P) = \mathbb{E}_P \left[ \|u - \phi(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right]$$

for the Bayes risk of an estimator $\phi \in \mathcal{M}$ under the distribution $P$. We denote the Wasserstein ball around $P_0$ as

$$W(\delta) = \{P \in \mathcal{P} : W(P, P_0) \leq \delta\}.$$

Then, denoting the Wasserstein balls around $P_0$ arising from perturbations in the first $N$ coordinates by

$$W_N(\delta) = \{P \in W(\delta) : \mathcal{L}^P((b, e_n)) = \mathcal{L}^{P_0}((b, e_n)) \text{ for } n > N\},$$

where $\mathcal{L}^P$ denotes the law under $P$. We have for any $N \geq 1$ that

$$\inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{P \in W(\delta)} \text{Obj}(\phi, P) \geq \inf_{\phi \in \mathcal{M}_{\text{aff}}} \sup_{P \in W(\delta)} \text{Obj}(\phi, P) \geq \inf_{\phi \in \mathcal{M}} \sup_{P \in W(\delta)} \text{Obj}(\phi, P) \geq \sup_{P \in W(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P) \geq \sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P). \quad (14)$$
Above, the first two inequalities follow from the inclusion $M_{\text{aff},N} \subset M_{\text{aff}} \subset M$, the third inequality follows from weak duality, and the last equality follows from the inclusion $W_N(\delta) \subset W(\delta)$. Finally, for any $P \in \mathcal{P}$ and $N \geq 1$, we denote the joint measure induced by projecting $b$ onto $\text{span}\{e_n\}_{n=1}^N$ whilst keeping $\varepsilon$ intact by

$$P^{(N)} := \mathcal{L}^P \left( \sum_{1 \leq n \leq N} e_n \langle b, e_n \rangle, \varepsilon \right).$$

(15)

Our proof consists of showing the following three claims:

**Claim 1**: The finite-dimensional version of strong duality holds, i.e.,

$$\inf_{\phi \in \mathcal{M}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P^{(N)}) = \inf_{\phi \in M_{\text{aff},N}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P^{(N)})$$

$$= \sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^{(N)}).$$

(16)

**Claim 2**: The truncation of $P$ to $P^{(N)}$ in the last term of (14) preserves the chain of inequalities, i.e.,

$$\sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P) \geq \sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^{(N)}).$$

(17)

**Claim 3**: The truncation of $P$ to $P^{(N)}$ in the first term of (14) has an error asymptotically negligible, i.e.,

$$\inf_{\phi \in M_{\text{aff},N}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P) - \inf_{\phi \in M_{\text{aff},N}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P^{(N)}) \leq o(1)$$

(18)

as $N \to \infty$. Combining the above three claims and the chain of inequalities (14), we conclude that

$$\inf_{\phi \in \mathcal{M}} \sup_{P \in W(\delta)} \text{Obj}(\phi, P) = \sup_{P \in W(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P)$$

(19)

by letting $N \to \infty$. $\Box$

We now provide the proofs of the three claims.

**Proof of Claim 1.** For $P \in \mathcal{P}$, we denote the marginal distribution of the first $N$ basis coefficients $\langle b, e_n \rangle$ and $\varepsilon$ by

$$Q^{(N)} := \mathcal{L}^P \left( (\langle b, e_1 \rangle, \cdots, \langle b, e_N \rangle, \varepsilon) \right).$$

(20)

Note that $Q^{(N)}$ is a probability measure on $\mathbb{R}^{N+m}$, while the distribution $P^{(N)}$ is supported on $C(D) \times \mathbb{R}^m$. In particular, we have $Q^{(N)}_0 := \mathcal{L}^b \left( (\langle b, e_1 \rangle, \cdots, \langle b, e_N \rangle, \varepsilon) \right)$ is a multivariate Gaussian. Now, for the weighted cost function

$$c_N(r,s) = \sum_{n=1}^N (r_n - s_n)^2 w_n + \sum_{j=1}^m (r_{N+j} - s_{N+j})^2 \quad \forall r,s \in \mathbb{R}^{N+m}$$

we have

$$\inf_{\phi \in M_{\text{aff},N}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P) = \sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P)$$

(21)
on $\mathbb{R}^{N+m}$, we denote the corresponding optimal transport cost between probability measures $\tau$ and $\nu$ on $\mathbb{R}^{N+m}$ by

$$W_2^N(\tau, \nu) = \min_{\pi: \pi r = \tau, \pi s = \nu} \mathbb{E}_{(R,S) \sim \pi}[c_N(R, S)],$$

where we imposed $\pi$ to be a probability measure implicitly to avoid cluttered notations. Thus, by writing the shorthand

$$g(r) := \left\| \sum_{n=1}^{N} r_n T(e_n) - \phi \left( \left( \sum_{n=1}^{N} r_n T(e_n) (x_j) + r_{N+j} \right)_{j=1}^{m} \right) \right\|_2^2,$$

we obtain that

$$\sup_{P \in \mathcal{W}_N(\delta)} \text{Obj}(\phi, P^{(N)}) = \sup_{Q^{(N)}: \mathbb{W}_N(Q^{(N)}, Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)].$$

Assume momentarily that $\phi \in \mathcal{M}_{\text{aff}, N}$. In this case, $g$ is a convex (non-constant) quadratic function and [7, Theorem 1] implies the dual formulation

$$\sup_{Q^{(N)}: \mathbb{W}_N(Q^{(N)}, Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] = \inf_{\gamma \geq 0} \left( \gamma \delta^2 + \mathbb{E}_{R \sim Q_0^{(N)}} \left[ \sup_{s \in \mathbb{R}^{N+m}} \left( g(s) - \gamma c_N(R, s) \right) \right] \right).$$

(21)

The same theorem moreover implies that there exists a dual optimizer $\gamma^*$ to the right-hand side minimization problem of (21). Since the distributions in the set

$$\{ Q^{(N)}: \mathbb{W}_N(Q^{(N)}, Q_0^{(N)}) \leq \delta \}$$

are uniformly bounded in the second moment and $g$ is quadratic in $r$, we have that

$$\sup_{Q^{(N)}: \mathbb{W}_N(Q^{(N)}, Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] < \infty.$$

Since also $\sup_{s \in \mathbb{R}^{N+m}} g(s) = \infty$, we have necessarily that $\gamma^* > 0$.

Observe that $g(r)$ can be written in the form $g(r) = r^T G r + c^T r + \|a_0\|_2^2$ for some $G \in \mathbb{S}_{N+m}^+$ and $c \in \mathbb{R}^{N+m}$, where we denote $\mathbb{S}_{N+m}^+$ as the set of positive semi-definite matrices with a dimension of $N + m$. Denoting

$$W_N = \text{diag}(w_1, \ldots, w_N, 1, \ldots, 1),$$

then, almost surely for $R \sim Q_0^{(N)}$, we have

$$g(s) - \gamma^* c_N(R, s) = s^T (G - \gamma^* W_N) s + (2\gamma^* R^T W_N + c^T) s + \|a_0\|_2^2 + \gamma^* R^T W_N R.$$
Since $R$ follows a non-degenerate multivariate Gaussian distribution, we have that necessarily $\gamma^* W_N - G \in \mathbb{S}^{N+m}_{++}$, otherwise $\sup_{s \in \mathbb{R}^{N+m}} g(s) - \gamma^* c_N(R, s) = \infty$ almost surely. Note that [7, Theorem 1] also implies that the optimal coupling between $Q_0^{(N)}$ and the maximizer to the left side of (21), if it exists, must be given as the law of $(R, s^*(R))$, for the affine push-forward map

$$s^*(R) = -\frac{1}{2}(G - \gamma^* W_N)^{-1}(2\gamma^* W_N R + c).$$

(22)

The existence of a solution $Q_\star^{(N)}$ to the left hand side of (21) as well as of an optimal coupling between $Q_0^{(N)}$ and $Q_\star^{(N)}$, which we denote by $\pi_\star$, can be verified by [15, Corollary 1(i)]. Indeed, since $\gamma^* W_N - G \in \mathbb{S}^{N+m}_{++}$, for the growth rate $\kappa$ defined to be

$$\kappa = \limsup_{r \to \infty} \frac{r^\top Gr}{r^\top W_N r},$$

we have that $\kappa < \gamma^*$. By the affine push-forward map (22), $Q_\star^{(N)}$ is also Gaussian, whence we may write (21) as

$$\sup_{Q^{(N)}, W_N(Q^{(N)}, 0^{(N)})} \mathbb{E}_{R \sim Q^{(N)}}[g(R)] = \sup_{Q^{(N)}, W_N(Q^{(N)}, 0^{(N)}) \leq \delta Q^{(N)} \text{ normal}} \mathbb{E}_{R \sim Q^{(N)}}[g(R)]$$

$$= \sup_{(\mu, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma + \mu \mu^\top \rangle + \|\alpha_0\|_{L^2(D)}^2$$

$$\geq \sup_{(\mu, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma + \mu \mu^\top \rangle,$$

where the last inequality is because $c^\top \mu \geq 0$ after a possible sign change in $\mu$. Here $\mathcal{S}_N$ is a compact and convex set coming from a modified Gelbrich distance

$$\mathcal{S}_N = \left\{ (\mu, \Sigma) : \|\mu\|_2^2 + tr(W_N \Sigma) + tr(W_N \Sigma_0) - 2tr\left(\sqrt{\Sigma_0 W_N \Sigma W_N \Sigma_0} \right)^{1/2} \leq \delta^2 \right\},$$

where $\Sigma_0 \in \mathbb{S}^{N+m}_{++}$ is the covariance matrix of $Q_0^{(N)}$. We show in passing how the modified Gelbrich distance arises. The usual squared-Euclidean cost function between $r$ and $s \in \mathbb{R}^{N+m}$ is $\|r - s\|_2^2$, which gives rise to the usual Gelbrich distance [28, Proposition 2.2] that coincides with the type-2 Wasserstein distance between multivariate Gaussians. Herein, our new cost is $(r - s)^\top W_N (r - s)$, thus the optimal coupling $\pi_\star$ for the new cost solves

$$\min_{\pi : \pi_{r=r_, s=s} = \nu} \left(-\int r^\top W_N s d\pi(r, s)\right).$$

Using substitution of variables $\tilde{r} = \sqrt{W_N} r$ and $\tilde{s} = \sqrt{W_N} s$, we find that the above problem reduces to the optimal transport problem with a squared-Euclidean cost.
In the sequel we denote the Wasserstein balls around $P_0$ arising from perturbations in the first $N$ coordinates and restricting to the family of Gaussian distributions as

$$\mathcal{W}_{\text{nor},N}(\delta) = \{ P \in \mathcal{W}_N(\delta) : Q^{(N)} \text{ is centered full-rank normal} \}.$$ 

Therefore, we obtain

$$\inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{\alpha_0 = 0} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] \geq \inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] \geq \inf_{\phi \in \mathcal{M}_{\text{aff},N}, (\mu, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma + \mu \mu^T \rangle$$

$$= \inf_{\phi \in \mathcal{M}_{\text{aff},N}, (\mu, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma \rangle = \inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \sup_{(0, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma \rangle \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)],$$

where the last equality is because $s^*(R)$ is zero-mean whenever $c = 0$, which in turn follows from $\alpha_0 = 0$. Hence all inequalities become equalities, and we conclude that

$$\inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] = \inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \sup_{(0, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma \rangle.$$ 

Remind that the matrix $G$ is dependent on the coefficients of the affine estimator $\phi$. By Sion’s minimax theorem [29], we have

$$\inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \sup_{(0, \Sigma) \in \mathcal{S}_N} \langle G, \Sigma \rangle = \sup_{(0, \Sigma) \in \mathcal{S}_N} \inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \langle G, \Sigma \rangle \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta, Q^{(N)} \text{ is centered full-rank normal}} \mathbb{E}_{R \sim Q^{(N)}} [g(R)].$$

The last “full-rank” assertion comes from the fact that $s^*(R)$ is a non-degenerate linear transformation of $R$, and that a linear transformation of a multivariate Gaussian is also Gaussian. Thus

$$\inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{P \in \mathcal{W}_N(\delta)} \text{Obj}(\phi, P^{(N)}) = \inf_{\phi \in \mathcal{M}_{\text{aff},N}} \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)] = \inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \sup_{Q^{(N)}:W_N(Q^{(N)},Q_0^{(N)}) \leq \delta} \mathbb{E}_{R \sim Q^{(N)}} [g(R)]$$

$$= \sup_{P \in \mathcal{W}_{\text{nor},N}(\delta)} \inf_{\phi \in \mathcal{M}_{\text{aff},N}, \alpha_0 = 0} \text{Obj}(\phi, P^{(N)}).$$
For $\mathbb{W}(P, P_0) \leq \delta$, note that $u$ is a process with continuous sample paths, whence we can interchange the integration
\[
E_P \left[\|u - \phi(Y_1, \ldots, Y_m)\|^2_{L^2(D)}\right] = E_P \left[\int_D |u(x) - \phi(Y_1, \ldots, Y_m)(x)|^2 \, dx\right]
= \int_D E_P \left[|u(x) - \phi(Y_1, \ldots, Y_m)(x)|^2\right] \, dx.
\]
Thus the optimal solution to the estimation problem
\[
\inf_{\phi \in \mathcal{M}} E_P \left[\|u - \phi(Y_1, \ldots, Y_m)\|^2_{L^2(D)}\right] = \int_D E_P \left[|u(x) - \phi(Y_1, \ldots, Y_m)(x)|^2\right] \, dx.
\] \tag{26}

is given by the conditional expectation function
\[
\phi(Y_1, \ldots, Y_m)(x) = E_P \left[u(x)|Y_1, \ldots, Y_m\right]. \tag{27}
\]

For any distribution $P$ that is a centered Gaussian random variable, it is easy to see that for $x \in D$, the random vector
\[
(u(x), Y_1, \ldots, Y_m) = (u(x), u(x_1) + \epsilon_1, \ldots, u(x_m) + \epsilon_m)
\]
is jointly Gaussian and the conditional expectation satisfies
\[
E_P \left[u(x)|Y_1, \ldots, Y_m\right] = (k_{\epsilon}(x, x_1), \ldots, k_{\epsilon}(x, x_m)) \cdot (K_{\epsilon})^{-1} \cdot (Y_1, \ldots, Y_m)^\top, \tag{28}
\]
where $k_{\epsilon}(x, x_j) = E_P[u(x)(u(x_j) + \epsilon_j)]$, and
\[
K_{\epsilon} = \left(E_P[(u(x_i) + \epsilon_i)(u(x_j) + \epsilon_j)]\right)_{ij} \in \mathbb{S}_+^m
\]
provided the matrix $K_{\epsilon}$ is invertible. Moreover, the optimal value of the Bayes risk \textsuperscript{(26)} is given by
\[
\int_D E_P\left[\text{Var}_P[u(x)|Y_1, \ldots, Y_m]\right] \, dx
= \int_D k(x, x) - (k_{\epsilon}(x, x_1), \ldots, k_{\epsilon}(x, x_m)) \cdot (K_{\epsilon})^{-1} \cdot (k_{\epsilon}(x, x_1), \ldots, k_{\epsilon}(x, x_m))^\top \, dx
\]
where $k(x, x) = E_P[u(x)u(x)]$. Thus
\[
\sup_{P \in \mathbb{W}_{\text{nor}, N}(\delta)} \inf_{\phi \in \mathcal{M}_{\text{aff}, N}, \alpha_0 = 0} \text{Obj}(\phi, P^{(N)}) = \sup_{P \in \mathbb{W}_{\text{nor}, N}(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^{(N)})
\leq \sup_{P \in \mathbb{W}_{\text{N}}(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^{(N)}),
\]
On the other hand,
\[
\sup_{P \in W_N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P) \leq \inf_{\phi \in \mathcal{M}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P) \leq \inf_{\phi \in \mathcal{M}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P).
\]
Thus combining the above chains of inequalities and the equality (25), we have
\[
\inf_{\phi \in \mathcal{M}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P) = \inf_{\phi \in \mathcal{M}} \sup_{P \in W_N(\delta)} \text{Obj}(\phi, P) = \sup_{P \in W_nor,N(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P).
\]
Thus we have established (16).

**Proof of Claim 2.** By the proof of Claim 1, there exists a Nash equilibrium of (16), which we denote by \((\phi^*_N, P^*_N)\). In particular, by previous Claim 1, we can choose \(\phi^*_N\) as affine and \(Q_N^* = \mathcal{L}^P_N(\{\langle b, e_n \rangle \}_{n=1}^{N} + \epsilon)\) as some centered full-rank normal distribution. Also, the pair \((\phi^*_N, Q_N^*)\) is the unique Nash equilibrium corresponding to the game (23) and (24). Moreover, under the law \(P_N^*\), the random elements
\[
\{\{\langle b, e_n \rangle \}_{n=1}^{N}\} \quad \text{and} \quad \{\{b, e_n\}\}_{n=N+1}^{\infty}
\]
are independent. Finally, we have that
\[
\mathcal{L}^P_N(\{\{b, e_n\}\}_{n=N+1}^{\infty}) = \mathcal{L}^{P_0}(\{\{b, e_n\}\}_{n=N+1}^{\infty}).
\]
Note that \(P_N^*\) is a Borel-measurable Gaussian random variable on \(C(D)\). We now show our claim (17). Note that
\[
Y_j = u(x_j) + \epsilon_j = \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j + \left( u(x_j) - \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) \right),
\]
where the last term (denoted by \(R_{j,N}\) as a shorthand) is of zero-mean under \(P_N^*\). Thus any affine estimator \(\phi\) can be written as
\[
\phi(Y_1, \ldots, Y_m) = \sum_{j=1}^{m} \alpha_j \left( \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right) + \sum_{j=1}^{m} \alpha_j R_{j,N}.
\]
Let \(\{\bar{e}_k\}_{k=1}^{\infty}\) be the Gram-Schmidt orthonormalization of \(\{T(e_k)\}_{k=1}^{\infty}\). In the process of orthonormalizing \(\{T(e_k)\}_{k=1}^{\infty}\), for any \(n\) such that the function \(T(e_n)\) is already included in
the span of \( \{ T(e_k) \}_{k=1}^{n-1} \), we define \( \tilde{e}_n \) as the zero function. Note that the functions \( \{ \tilde{e}_k \}_{k=1}^\infty \)
do not necessarily constitute a basis of \( L_2(D) \). We have

\[
\sup_{P \in W_N(\delta)} \inf_{\phi \in M} \text{Obj}(\phi, P) \\
\geq \inf_{\phi \in M} \text{Obj}(\phi, P_N^*) \\
= \inf_{\phi \in M} \mathbb{E}_{P_N^*} \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right] \\
= \inf_{\phi \in M} \mathbb{E}_{P_N^*} \left[ \| u - \phi(Y_1, \ldots, Y_m) \|_{L^2(D)}^2 \right] \quad \text{due to Gaussianity} \\
= \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^\infty \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
\geq \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
\geq \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
= \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
= \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
= \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
\geq \inf_{\phi \in M_{\text{aff}}} \mathbb{E}_{P_N^*} \left[ \sum_{n=1}^N \langle u - \phi(Y_1, \ldots, Y_m), \tilde{e}_n \rangle^2 \right] \\
= \sup_{P \in W_N(\delta)} \inf_{\phi \in M} \text{Obj}(\phi, P^{(N)}).
\]
The penultimate equality is because that
\[ \mathbb{E}_{P_N^*} \left( \left\langle u - \sum_{j=1}^{m} \alpha_j \left( \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle \right) \] 
\[ = \mathbb{E}_{P_N^*} \left( \left\langle u - \sum_{j=1}^{m} \alpha_j \left( \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle \right) \] 
\[ = 0, \]
where we have used the independence in (30) and the fact that \( R_j,N \) have zero mean.

Therefore, we have established Claim 2.

**Proof of Claim 3.** Since \( \phi_N^* \) is affine, we can write \( \phi_N^* \) in the form \( \phi_N^*(Y_1, \ldots, Y_m) = \sum_{j=1}^{m} \alpha_j^* Y_j \), where \( \alpha_j^* \in \text{span} \{ T(e_k) \}_{k=1}^N \). Here, we have suppressed the dependence of \( \alpha_j^* \) on \( N \) to simplify the notations. Similar to the proof of Claim 2, we let \( \{ \tilde{e}_k \}_{k=1}^\infty \) be the Gram-Schmidt orthonormalization of \( \{ T(e_k) \}_{k=1}^\infty \). Also note that there exists a constant \( C \) independent of \( N \), such that for any \( 1 \leq j \leq m \),
\[ \| \alpha_j^* \|_{L^2(D)}^2 = \sum_{n=1}^{N} |\langle \alpha_j^*, \tilde{e}_n \rangle|^2 \leq C < \infty. \]

This is because we can choose \((0, \Sigma) \in S_N\) in the inner constraint of (23) to be the nominal measure, and thereby conclude that the optimal objective value in (23) is lower bounded by \( C' \sum_{j=1}^{m} \| \alpha_j \|_{L^2(D)}^2 \), for some constant \( C' \) independent of \( N \). For any \( N \), we have
\[ \sup_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi_N^*, P) - \sup_{P \in \mathcal{W}_N(\delta)} \text{Obj}(\phi_N^*, P(N)) \]
\[ = \sup_{P \in \mathcal{W}(\delta)} \left( \sum_{n=1}^{N} \mathbb{E}_P(\langle u - \phi_N^*, \tilde{e}_n \rangle)^2 + \sum_{n=N+1}^{\infty} \mathbb{E}_P(\langle u, \tilde{e}_n \rangle)^2 \right) \]
\[ - \sup_{P \in \mathcal{W}_N(\delta)} \sum_{n=1}^{N} \mathbb{E}_P(N)(\langle u - \phi_N^*, \tilde{e}_n \rangle)^2 \]
\[ \leq \sup_{P \in \mathcal{W}(\delta)} \sum_{n=1}^{N} \mathbb{E}_P(\langle u - \phi_N^*, \tilde{e}_n \rangle)^2 - \sup_{P \in \mathcal{W}_N(\delta)} \sum_{n=1}^{N} \mathbb{E}_P(N)(\langle u - \phi_N^*, \tilde{e}_n \rangle)^2 \]
\[ + \sup_{P \in \mathcal{W}(\delta)} \sum_{n=N+1}^{\infty} \mathbb{E}_P(\langle u, \tilde{e}_n \rangle)^2. \] (31)
For the last term in (31), note that
\[
\sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P \left[ \sum_{n=N+1}^{\infty} ((u_n, \tilde{e}_n))^2 \right]
\]
\[
\leq 2 \mathbb{E}_{P_0} \left[ \sum_{n=N+1}^{\infty} ((u_0, \tilde{e}_n))^2 \right] + 2 \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \sum_{n=N+1}^{\infty} ((u - u_0, \tilde{e}_n))^2 \right]
\]
\[
\leq o(1) + O(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \|u - u_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n \|_{L^2(D)}^2 \right],
\]
where \( \pi \) is the optimal coupling between the marginals \( P_0 \) and \( P \), and
\[
\sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \|T(b - b_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n)\|_{L^2(D)}^2 \right]
\]
\[
\leq O(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \|T(b - b_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n)\|_{H^0}^2 \right]
\]
\[
\leq O(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \|b - b_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n\|_{H^0}^2 \right]
\]
\[
\leq o(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \|b - b_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n\|_{H^w}^2 \right]
\]
\[
\rightarrow 0 \text{ as } N \rightarrow \infty,
\]
where the second inequality comes from Assumption 2.3(ii), while the third inequality comes from Assumption 2.4 and the fact that \( b - b_0 - \sum_{n=1}^{N} \langle b - b_0, e_n \rangle e_n \) is in the space spanned by \( \{e_n\}_{n=N+1}^{\infty} \). For the first two terms in (31), we write
\[
\phi_N^*(Y_1, \ldots, Y_m) = \sum_{j=1}^{m} \alpha_j^* \left( \sum_{k=1}^{N} \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right) + \sum_{j=1}^{m} \alpha_j^* R_j,N.
\]
Thus for any feasible $P$ in $W(\delta)$, we have
\[
\mathbb{E}_P(\langle u - \phi^*_N, \tilde{e}_n \rangle)^2
= \mathbb{E}_P \left( \left\langle u - \sum_{j=1}^m \alpha_j^*(x) \left( \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle^2 \right)
- 2\mathbb{E}_P \left( \left\langle u - \sum_{j=1}^m \alpha_j^*(x) \left( \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle \left\langle \sum_{j=1}^m \alpha_j^*(x) R_{j,N}, \tilde{e}_n \right\rangle \right)
+ \mathbb{E}_P \left( \sum_{j=1}^m \alpha_j^*(x) R_{j,N}, \tilde{e}_n \right)^2.
\]

Note that
\[
\sum_{n=1}^N \mathbb{E}_P \left( \left\langle u - \sum_{j=1}^m \alpha_j^*(x) \left( \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle^2 \right)
\leq \sup_{P \in W_N(\delta)} \sum_{n=1}^N \mathbb{E}_{P^N}(\langle u - \phi^*_N, \tilde{e}_n \rangle)^2.
\]

Also, by Cauchy-Schwarz, we obtain
\[
\sum_{n=1}^N \mathbb{E}_P \left( \left\langle u - \sum_{j=1}^m \alpha_j^*(x) \left( \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle \left( \sum_{j=1}^m \alpha_j^*(x) R_{j,N}, \tilde{e}_n \right) \right)
\leq \sqrt{\mathbb{E}_P \left( \sum_{n=1}^N \left\langle u - \sum_{j=1}^m \alpha_j^*(x) \left( \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) + \epsilon_j \right), \tilde{e}_n \right\rangle^2 \right)} \times \sqrt{\mathbb{E}_P \left( \sum_{n=1}^N \left( \sum_{j=1}^m \alpha_j^*(x) R_{j,N}, \tilde{e}_n \right)^2 \right)}
\leq \sqrt{\sup_{P \in W_N(\delta)} \sum_{n=1}^N \mathbb{E}_{P^N}(\langle u - \phi^*_N, \tilde{e}_n \rangle)^2} \sqrt{mC \left( \sum_{j=1}^m \mathbb{E}_P \left[ R_{j,N}^2 \right] \right)}.
\]
Therefore, denoting $\pi$ as the optimal coupling between $P$ and $P_0$, we have

$$
\sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P (R_{j,N})^2
= \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P \left( u(x_j) - \sum_{k=1}^N \langle b, e_k \rangle T(e_k)(x_j) \right)^2
\leq 2 \mathbb{E}_{P_0} \left( u^0(x_j) - \sum_{k=1}^N \langle b^0, e_k \rangle T(e_k)(x_j) \right)^2
+ 2 \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left( u(x_j) - u^0(x_j) - \sum_{k=1}^N \langle b - b^0, e_k \rangle T(e_k)(x_j) \right)^2
\leq o(1) + 2 \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left( u(x_j) - u^0(x_j) - \sum_{k=1}^N \langle b - b^0, e_k \rangle T(e_k)(x_j) \right)^2.
$$

Moreover,

$$
\sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left( u(x_j) - u^0(x_j) - \sum_{k=1}^N \langle b - b^0, e_k \rangle T(e_k)(x_j) \right)^2
= \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \left( T(b - b^0 - \sum_{k=1}^N \langle b - b^0, e_k \rangle e_k)(x_j) \right)^2 \right]
\leq O(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \left\| T(b - b^0 - \sum_{k=1}^N \langle b - b^0, e_k \rangle e_k) \right\|_{H_\omega}^2 \right]
\leq O(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \left\| b - b^0 - \sum_{k=1}^N \langle b - b^0, e_k \rangle e_k \right\|_{H_\omega}^2 \right]
\leq o(1) \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_\pi \left[ \left\| b - b^0 \right\|_{H_\omega}^2 \right]
\rightarrow 0 \text{ as } N \rightarrow \infty,
$$

where the first inequality follows because $H_\omega$ is an RKHS consisting of continuous functions, so that point evaluations at the $x_j$’s are bounded, according to Assumption 2.3(ii). The second inequality also follows from Assumption 2.3(ii), while the third equality follows from Assumption 2.4. Finally, the last inequality follows because $\{e_n\}_{n=1}^\infty$ is an orthogonal
system. Therefore, we have that

\[ \sup_{P \in W(\delta)} \mathbb{E}_P (R_j,N)^2 \to 0 \text{ as } N \to \infty. \]

It then follows that

\[ \sup_{P \in W(\delta)} \text{Obj}(\phi^*_N, P) - \sup_{P \in W_N(\delta)} \text{Obj}(\phi^*_N, P^{(N)}) = o(1) \text{ as } N \to \infty, \]

establishing our Claim 3.

\[ \square \]

### 6.2 Proof of Proposition 3.1

**Proof of Proposition 3.1.** This is an immediate consequence of the inequality (14) and Claims 1-3 in the proof of Theorem 3.1.

\[ \square \]

### 6.3 Proof of Proposition 3.2

**Proof of Proposition 3.2.** Since the space \( C(D) \times \mathbb{R}^m \) is Polish, it suffices to show that the sequence \( P_N, N = 1, \ldots, \infty \) is tight. First note that \( P_0 \) is a finite Radon measure on \( C(D) \times \mathbb{R}^m \), and hence \( P_0 \) is tight. Therefore, for any \( 0 < \eta < 1 \), there exists a compact set \( C_0 \) in \( C(D) \times \mathbb{R}^m \), such that \( P_0(C_0) \geq 1 - \frac{\eta}{2} \). Now consider the set

\[ C_1 = \{ (b, \epsilon) \in C(D) \times \mathbb{R}^m : \exists (b^0, \epsilon^0) \in C_0, \| b - b^0 \|_{H_w}^2 + \| \epsilon - \epsilon^0 \|_2^2 \leq 2\delta^2/\eta \}, \]

which is compact since the space \( H_w \) is compactly embedded in \( C(D) \) by Assumption 2.2. Denote \( Q_N \) as the law of the difference \( (b - b^0, \epsilon - \epsilon^0) \) under the optimal coupling between \( (b, \epsilon) \sim P_N \) and \( (b^0, \epsilon^0) \sim P_0 \). Then,

\[ 1 - P_N(C_1) \leq 1 - P_0(C_0) + Q_N(\{ (b, \epsilon) \in H_w \times \mathbb{R}^m : \| b \|_{H_w}^2 + \| \epsilon \|_2^2 > 2\delta^2/\eta \}) \]

\[ \leq \frac{\eta}{2} + \frac{W^2(P_N, P_0)}{2\delta^2/\eta} \leq \frac{\eta}{2} + \frac{\eta}{2} = \eta, \]

where in the second inequality we used the Cauchy-Schwarz inequality. Therefore, we conclude that

\[ P_N(C_1) \geq 1 - \eta \quad \forall N, \]

and hence that the sequence \( P_N \) is tight. It follows that there exists a weakly convergent subsequence \( P_{N_l}, l \geq 1 \) with \( P_{N_l} \Rightarrow P_\infty \). Since the Wasserstein distance is lower semicontinuous, the limit \( P_\infty \) necessarily satisfies \( W(P_\infty, P_0) \leq \delta \).

\[ \square \]
6.4 Proof of Theorem 3.2

We start with a simple but useful result, which is well-known [38].

**Lemma 6.1** (Minimax theorem and Nash equilibrium). Let \( \phi^* \) be an optimal solution to the outer infimum of the problem

\[
\inf_{\phi \in \mathcal{M}} \sup_{P \in \mathcal{W}} \text{Obj}(\phi, P),
\]

and let \( P^* \) be an optimal solution to the outer supremum of the problem

\[
\sup_{P \in \mathcal{W}(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P).
\]

Then \((\phi^*, P^*)\) is a Nash equilibrium of (19).

**Proof of Lemma 6.1.** We have

\[
\sup_{P \in \mathcal{W}(\delta)} \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P) = \inf_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^*) \leq \text{Obj}(\phi^*, P^*) \leq \sup_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi^*, P).
\]

By the strong duality, all inequalities become equalities, thus we have

\[
\text{Obj}(\phi^*, P^*) = \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P^*) = \max_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi^*, P).
\]

This completes the proof. \( \qed \)

**Proof of Theorem 3.2.** Recall that we denote

\[
Q_N := \mathcal{L}^{P_N}((b, e_1), \cdots, (b, e_N), \epsilon)
\]

in the proof to Claim 2 of Theorem 3.1. We also denote additionally

\[
P^*_N := \mathcal{L}^{P^*_N}\left((\sum_{1 \leq n \leq N} e_n(b, e_n), \epsilon)\right).
\]

Letting \( k^{(N)}(x, x) = \mathbb{E}_{P_N^*}[u(x)^2] \), the objective value \( \text{Obj}(\phi_N^*, P_N^*) \) can be written as

\[
\text{Obj}(\phi_N^*, P_N^*) = \int_D \mathbb{E}_{P_N^*}[\text{Var}_{P_N^*}[u(x)|Y_1, \ldots, Y_m]]dx
\]

\[
= \int_D [k^{(N)}(x, x) - \left(k^{(N)}_e(x, x_1), \ldots, k^{(N)}_e(x, x_m)\right)^\top (K^{(N)}_e)^{-1} \left(k^{(N)}_e(x, x_1), \ldots, k^{(N)}_e(x, x_m)\right)]dx.
\]

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Thus the estimator $\phi_{\infty}^*$ is

$$\text{Obj}(\phi_{\infty}^*, P_{\infty}^*) = \int_{\mathcal{D}} \mathbb{E}_{P_{\infty}^*}[\text{Var}_{P_{\infty}^*}[u(x)|Y_1, \ldots, Y_m]] dx$$

$$= \int_{\mathcal{D}} k(x, x) - (k_c(x, x_1), \ldots, k_c(x, x_m)) \cdot (K_c)^{-1} \cdot (k_c(x, x_1), \ldots, k_c(x, x_m))' dx,$$

where $k(x, x) = \mathbb{E}_{P_{\infty}^*}[u(x)^2]$. Recall that $P_{N_l}^*$ is a (Gaussian) subsequence of $P_{N_l}^*$, which converges weakly to $P_{\infty}^*$. Note that $T$ is a bounded linear operator, and that the tail-difference in $P_{N_l}^*$ and $P_{N_l}^*$ is negligible. By [16, Exercise 2.1.4], convergence in distribution implies convergence of the second moment, thus uniformly for $x \in \mathcal{D}$, $k_{N_l}^*(x, x) \to k(x, x)$ and $k_{N_l}^*(x, x_i) \to k_c(x, x_i)$. Also, it holds that $K_{N_l}^* \to K_c$. Thus

$$\text{Obj}(\phi_{N_l}^*, P_{N_l}^*) = \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P_{N_l}^*) \to \text{Obj}(\phi_{\infty}^*, P_{\infty}^*) = \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P_{\infty}^*),$$

and hence that $P_{\infty}^*$ solves the right-hand side of (19).

We next show that $\phi_{\infty}^*$ solves the left-hand side of (19). We first note that due to the convergence of moments of $P_{N_l}^*$, it holds that

$$\lim_{l \to \infty} \phi_{N_l}^*(Y_1, \ldots, Y_m)(x) = \phi_{\infty}^*(Y_1, \ldots, Y_m)(x), \quad \forall Y_1, \ldots, Y_m \in \mathbb{R}, \quad x \in \mathcal{D},$$

Next, by Fatou’s lemma, we have that for any $P \in \mathcal{W}(\delta)$,

$$\mathbb{E}_P \left[ \|u - \phi_{\infty}^*(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right] \leq \liminf_{l \to \infty} \mathbb{E}_P \left[ \|u - \phi_{N_l}^*(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right].$$

Therefore,

$$\sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P \left[ \|u - \phi_{\infty}^*(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right] \leq \liminf_{l \to \infty} \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P \left[ \|u - \phi_{N_l}^*(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right].$$

Note that due to the finite-dimensional strong duality (16), $\phi_{N_l}^*$ also solves

$$\min_{\phi \in \mathcal{M}_{aff, N}} \max_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi, P^*(\mathcal{N})).$$

By (18) and strong duality, we have

$$\liminf_{N \to \infty} \sup_{P \in \mathcal{W}(\delta)} \mathbb{E}_P \left[ \|u - \phi_{N}^*(Y_1, \ldots, Y_m)\|_{L^2(\mathcal{D})}^2 \right] = \min_{\phi \in \mathcal{M}} \sup_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi, P).$$

Thus the estimator $\phi_{\infty}^*$ solves the min-max problem on the left-hand side of (19).
By Lemma 6.1 since \( \phi_\infty^* \) has to solve \( \min_{\phi \in \mathcal{M}} \text{Obj}(\phi, P_\infty^*) \), we have that \( \phi_\infty^* \) is uniquely determined (independent of the choice of the subsequence \( \phi_{N_i}^* \)), thus

\[
\lim_{N \to \infty} \phi_N^*(Y_1, \ldots, Y_m)(x) = \phi_\infty^*(Y_1, \ldots, Y_m)(x) \quad \forall \ Y_1, \ldots, Y_m \in \mathbb{R}, \quad x \in \mathcal{D}.
\]

Moreover, by Lemma 6.1, \( P_\infty^* \) has to solve \( \max_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi_\infty^*, P) \). We show in the sequel that \( P_\infty^* \) is uniquely determined (independent of the choice of the subsequence \( P_{N_i}^* \)), from which the sequence \( P_N^* \) converges to \( P_\infty^* \) in the weak topology as a whole. By Theorem 1 in [7], we have the reformulation

\[
\max_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi_\infty^*, P) = \inf_{\gamma \geq 0} \left( \gamma \delta^2 + \mathbb{E}_{P_0} \left[ \sup_{(b, \epsilon) \in C(\mathcal{D}) \times \mathbb{R}^m} \left( \|T(b) - \phi_\infty^*((T(b)(x_i) + \epsilon_i)i)\|_{L^2(\mathcal{D})}^2 - \gamma(\|b - b^0\|_{H_w}^2 + \|\epsilon - \epsilon^0\|_2^2) \right) \right] \right).
\]

We claim that the optimal dual \( \gamma^* \) is sufficiently large so that

\[
\|T(b) - \phi_\infty^*((T(b)(x_i) + \epsilon_i)i)\|_{L^2(\mathcal{D})}^2 - \gamma^*(\|b - b^0\|_{H_w}^2 + \|\epsilon - \epsilon^0\|_2^2) < 0 \quad \forall \ (b, \epsilon) \in H_w \times \mathbb{R}^m \quad \text{and} \quad (b, \epsilon) \neq 0.
\]

(32)

It is easy to see that \( \gamma^* > 0 \). Suppose that (32) does not hold, then

\[
\|T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon^*_i)i), T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon^0_i)i) \neq 0,
\]

for some \( (b^*, \epsilon^*) \neq 0 \). Then for all \( (b^0, \epsilon^0) \in C(\mathcal{D}) \times \mathbb{R}^m \) satisfying

\[
\langle T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon^*_i)i), T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon^0_i)i) \neq 0,
\]

we have that

\[
\sup_{(b, \epsilon) \in C(\mathcal{D}) \times \mathbb{R}^m} \left( \|T(b) - \phi_\infty^*((T(b)(x_i) + \epsilon_i)i)\|_{L^2(\mathcal{D})}^2 - \gamma^*(\|b - b^0\|_{H_w}^2 + \|\epsilon - \epsilon^0\|_2^2) \right)
\]

\[
\geq \sup_t \left( \|t(T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon^*_i)i)) + (T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon^0_i)i)) \|_{L^2(\mathcal{D})}^2 \right)
\]

\[
- t^2\gamma^*(\|b^*\|_{H_w}^2 + \|\epsilon^*\|_2^2)
\]

\[
\geq \sup_t t^2 \left( \|T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon^*_i)i)\|_{L^2(\mathcal{D})}^2 - \gamma^*(\|b^*\|_{H_w}^2 + \|\epsilon^*\|_2^2) \right)
\]

\[
+ 2t\langle T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon^*_i)i), T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon^0_i)i) \rangle
\]

\[
+ \|T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon^0_i)i)\|_{L^2(\mathcal{D})}^2 = \infty,
\]

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where the infinite optimal value is due to the nonnegativity of the coefficient associated with the quadratic term \( t^2 \). Moreover, observe that the constraint

\[
\langle T(b^*) - \phi_\infty^*((T(b^*)(x_i) + \epsilon_i^*)_i), T(b^0) - \phi_\infty^*((T(b^0)(x_i) + \epsilon_0^*)_i) \rangle = 0
\]

is a linear constraint in \((b^0, \epsilon^0)\), and that \((b^0, \epsilon^0)\) cannot take the value \((b^*, \epsilon^*)\). Thus the collection of \((b^0, \epsilon^0)\) satisfying (33) is a subset of a proper linear subspace of \( C(D) \times \mathbb{R}^m \). This collection is closed because \( T : C(D) \to C(D) \) is bounded. Thus event (33) has probability strictly less than one. This concludes the proof of claim (32).

Denoting the shorthand

\[
J(b, \epsilon) = \|T(b) - \phi_\infty^*((T(b)(x_i) + \epsilon_i)_i)\|_{L^2(D)}^2 - \gamma^* (\|b - b^0\|_{H^\omega}^2 + \|\epsilon - \epsilon^0\|_2^2)
\]

any maximizer of \( J \) has to satisfy the first-order optimality condition

\[
\left. \frac{\partial}{\partial t} J(b + th_b, \epsilon + th_\epsilon) \right|_{t=0} = 0 \quad \forall (h_b, h_\epsilon) \in C(D) \times \mathbb{R}^m.
\]

It is easy to compute that

\[
\left. \frac{1}{2} \frac{\partial}{\partial t} J(b + th_b, \epsilon + th_\epsilon) \right|_{t=0} = \langle T(b) - \phi_\infty^*((T(b)(x_i) + \epsilon_i)_i), T(h_b) - \phi_\infty^*((T(h_b)(x_i) + (h_\epsilon)_i)_i) \rangle
\]

\[
- \gamma^* \left\{ (b - b^0, h_b)_{H^\omega} + (\epsilon - \epsilon^0, h_\epsilon) \right\}.
\]

Suppose that \((b, \epsilon)\) and \((\tilde{b}, \tilde{\epsilon})\) are two maximizers of \( J \), by choosing \((h_b, h_\epsilon) = (b - \tilde{b}, \epsilon - \tilde{\epsilon})\), we have

\[
\|T(h_b) - \phi_\infty^*((T(h_b)(x_i) + (h_\epsilon)_i)_i)\|_{L^2(D)}^2 - \gamma^* (\|h_b\|_{H^\omega}^2 + \|h_\epsilon\|_2^2) = 0.
\]

From our earlier claim (32), we conclude that \((b, \epsilon) = (\tilde{b}, \tilde{\epsilon})\). By Theorem 1 in [7], this shows that the solution to \( \max_{P \in \mathcal{W}(\delta)} \text{Obj}(\phi_\infty^*, P) \) is unique.

\[\square\]

### 6.5 Proof of Proposition 3.3

*Proof of Proposition 3.3.* First, suppose that the following statement holds true:

“\( K_\epsilon \) is invertible for the limit \( P_\infty^* \) of some weakly convergent subsequence of \( P_N^* \)”.

Then by Theorem 3.2, the sequence \( P_N^* \) weakly converges to \( P_\infty^* \) as a whole. Since the sequence \( P_N^* \) is Gaussian, we have \( \det(K_\epsilon^{(N)}) \to \det(K_\epsilon) \neq 0 \) as \( N \to \infty \).
Next, suppose that condition (34) does not hold, and suppose that \( \det(K^{(N)}) \) does not converge to 0 as \( N \to \infty \). Then there exists a subsequence of \( P^*_N \), denoted by \( P^*_{N_l} \), \( l \geq 1 \), such that the sequence of determinants \( \det(K^{(N_l)}) \) is uniformly bounded away from 0. Furthermore, \( P^*_{N_l} \) has a weak limit (upon passing into a further subsequence, e.g., by Proposition 3.2). It is clear that condition (34) applies to this subsequence \( P^*_{N_l} \), which is a contradiction! \( \square \)

6.6 Proof of Lemma 3.3

**Proof of Lemma 3.3**. Let \( P \) be such that \( W(P, P_0) \leq \delta \). To show that the matrix in question is strictly positive definite, it suffices to show that

\[
\inf_{\xi \in \mathbb{R}^d : \|\xi\|_2 = 1} \|\xi\|_2^2 = \inf_{\xi \in \mathbb{R}^d : \|\xi\|_2 = 1} \mathbb{E}_P \left[ \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) \right]^2 > 0.
\]

To this end, let \( \pi \) be a coupling such that

\[
\mathbb{E}_\pi \left[ c((b, \epsilon), (b^0, \epsilon^0)) \right] = \mathbb{E} \left[ \|\epsilon - \epsilon^0\|_2^2 + \|b - b^0\|_{H_w}^2 \right] \leq \delta^2,
\]

where the marginal distribution of \((b, \epsilon)\) and \((b^0, \epsilon^0)\) are \( P \) and \( P_0 \), respectively. We denote \( u = T(b) \) and \( u^0 = T(b^0) \). Let \( C_m \) be the constant such that (due to the RKHS property of \( H_w \))

\[
|f(x_i)| \leq C_m \|f\|_{H_w} \quad \forall f \in H_w, \ i = 1, \ldots, m.
\]

By Fatou’s lemma

\[
\mathbb{E}_\pi \left[ (u(x_i) - u^0(x_i))^2 \right] \leq \liminf_{N \to \infty} \mathbb{E}_\pi \left[ \left( \sum_{k=1}^{N} \langle b - b^0, e_k \rangle T(e_k)(x_i) \right)^2 \right]
\]

\[
= \liminf_{N \to \infty} \mathbb{E}_\pi \left[ \left( T \left( \sum_{k=1}^{N} \langle b - b^0, e_k \rangle e_k \right)(x_i) \right)^2 \right]
\]

\[
\leq C_m^2 \liminf_{N \to \infty} \mathbb{E}_\pi \left[ \left\| \sum_{k=1}^{N} \langle b - b^0, e_k \rangle e_k \right\|_{H_w}^2 \right]
\]

\[
\leq C_m^2 C_w^2 \liminf_{N \to \infty} \mathbb{E}_\pi \left[ \left\| \sum_{k=1}^{N} \langle b - b^0, e_k \rangle e_k \right\|_{H_w}^2 \right]
\]

\[
\leq C_m^2 C_w^2 \tilde{C} \liminf_{N \to \infty} \mathbb{E}_\pi \left[ \left\| b - b^0 \right\|_{H_w}^2 \right] = (35),
\]

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where the constant $C_{\tilde{w}}$ is from Assumption 2.3(ii), and the constant $\tilde{C}$ is due to Assumption 2.4.

For any $\xi \in \mathbb{R}^d$ with $\|\xi\|_2 = 1$,

$$E_{\pi} \left[ \left( \sum_{i=1}^{m} \xi_i (u^0(x_i) + \epsilon_i^0) \right)^2 \right]$$

$$= E_{\pi} \left[ \left( \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) + \sum_{i=1}^{m} \xi_i (u^0(x_i) - u(x_i) + \epsilon_i^0 - \epsilon_i) \right)^2 \right]$$

$$\leq 2E_{\pi} \left[ \left( \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) \right)^2 \right] + 4E_{\pi} \left[ \left( \sum_{i=1}^{m} \xi_i (u^0(x_i) - u(x_i)) \right)^2 \right]$$

$$+ 4E_{\pi} \left[ \left( \sum_{i=1}^{m} \xi_i (\epsilon_i^0 - \epsilon_i) \right)^2 \right]$$

$$\leq 2E_{P} \left[ \left( \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) \right)^2 \right] + 4E_{\pi} \left[ \sum_{i=1}^{m} (u(x_i) - u(x_i))^2 \right] + 4E_{\pi} [\|\epsilon^0 - \epsilon\|^2]$$

$$\leq 2E_{P} \left[ \left( \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) \right)^2 \right] + O(1)\delta^2,$$

where we used the previous inequality (35) to estimate $E_{\pi} \left[ \sum_{i=1}^{m} (u^0(x_i) - u(x_i))^2 \right]$. Note that $(E_{P_0}[Y_i Y_j])_{ij} \geq \sigma^2 I_{m \times m}$, since $\epsilon_i^0$ are independent $\mathcal{N}(0,\sigma^2)$ noise under $P_0$. Therefore,

$$\inf_{\xi \in \mathbb{R}^d, \|\xi\|_2 = 1} E_{P} \left[ \left( \sum_{i=1}^{m} \xi_i (u(x_i) + \epsilon_i) \right)^2 \right] \geq \frac{1}{2} \sigma^2 - O(1)\delta^2 > 0,$$

for all $\delta < \delta_0$, where $\delta_0$ is a positive constant that depends on $T, m, (x_i), \mathcal{H}_w, \mathcal{H}_{\tilde{w}}$ and $\sigma^2$.

### 6.7 Proof of Theorem 3.4

The proof for the inverse problem works verbatim as the proof to Theorem 3.1 with minor modifications. For example, instead of considering $\text{coef}(\phi) \in \text{span}\{T(e_n)\}_{n=1}^N$, we consider $\text{coef}(\phi) \in \text{span}\{e_n\}_{n=1}^N$. We suppress details to avoid repetitions.