Universal Robust Regression via Maximum Mean Discrepancy

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Many modern datasets are collected automatically and are thus easily contaminated by outliers. This led to a regain of interest in robust estimation, including new notions of robustness such as robustness to adversarial contamination of the data. However, most robust estimation methods are designed for a specific model. Notably, many methods were proposed recently to obtain robust estimators in linear models (or generalized linear models), and a few were developed for very specific settings, for example beta regression or sample selection models. In this paper we develop a new approach for robust estimation in arbitrary regression models, based on Maximum Mean Discrepancy minimization. We build two estimators which are both proven to be robust to Huber-type contamination. We obtain a non-asymptotic error bound for one them and show that it is also robust to adversarial contamination, but this estimator is computationally more expensive to use in practice than the other one. As a by-product of our theoretical analysis of the proposed estimators we derive new results on kernel conditional mean embedding of distributions which are of independent interest.

1. Introduction

Robustness is a fundamental problem in statistics, which aims at using statistical procedures that remain stable in presence of outliers. Historically, outliers were mistakes in data collection, or observations of individuals belonging to a different population than the population of interest. Robustness became even more important in the modern context where automatically collected datasets are often heterogeneous. Moreover, some strategic datasets are susceptible of malevolent manipulations.

In the statistical literature, the development of robust estimation methods for regression models generally focusses on the construction of Z-estimators (Van der Vaart, 2000, Chapter 5) for which each individual observation can only have a bounded impact on the estimating equations, and which therefore have a bounded influence func-
tion (Hampel, 1974a,b). This strategy has been successfully applied for the robust estimation of the regression coefficients in generalized linear models (Künsch et al., 1989; Cantoni and Ronchetti, 2001, 2006) as well as e.g. robust inference in the negative binomial regression model with unknown overdispersion parameter (Aeberhard et al., 2014) and in the Heckman sample selection model (Zhelonkin et al., 2016). Based on other approaches, robust estimators for mixtures of linear regression models (see e.g. Bai et al., 2012), for the Beta regression model with unknown precision parameter (Ghosh, 2019) and for robust linear least squares regression (Audibert and Catoni, 2011) have been developed.

In the past ten years there was a renewed interest for robust methods in the machine learning community. Catoni (2012) developed a loss function whose minimization leads to robust estimators of the expectation of a random variable, a technique which was then adapted to many situations including linear regression (Catoni and Giulini, 2017). More generally, Lipschitz loss functions, such as the absolute loss or Huber’s loss (Huber, 1992), lead to robustness of the empirical risk minimization procedure, a fact that was used in Chinot et al. (2020b); Alquier et al. (2019); Chinot et al. (2020a); Holland (2019) to study robust procedures of classification and regression. The Median-of-Means approach of Nemirovskij and Yudin (1983); Devroye et al. (2016) was also adapted to various machine learning problems (Lugosi and Mendelson, 2019); Lecué and Lerasle, 2019; Lugosi and Mendelson, 2019a; Depersin, 2020; Lecué et al. 2020; Lecué and Lerasle, 2020), including least squares regression, logistic regression, quantile regression and classification under various losses.

In the discussion by Sture Holm in Bickel et al. (1976), as well as in Parr and Schucany (1980), minimum distance estimation is identified as a way to obtain robust estimators. Building on this idea, Basu et al. (1998) introduced a density power divergence minimization approach for robust inference in parametric models for i.i.d. observations. This procedure is extended to regression models in Ghosh and Basu (2013) but suffers from two limitations. Firstly, the optimization of the objective function is, in general, a computationally challenging problem. Secondly, there is no general result which guarantees that the resulting $M$-estimator is robust. Its influence function is however known to be bounded for the Gaussian linear regression model (Ghosh and Basu, 2013), for the Poisson and logistic regression models (Ghosh and Basu, 2016) and for the Beta regression model with unknown precision parameter (Ghosh and Basu, 2013).

In this paper we introduce a new minimum distance estimation strategy for parameter inference in regression models which (a) is proven to be robust to outliers, both in the fixed and random design setting, under general conditions on the statistical model and (b) only requires to be able to sample from the model and to compute the gradient of its log-likelihood function to be applicable. In this sense, the approach proposed in this work defines a universal robust regression method. More specifically, we present in this paper a minimum distance estimation procedure for regression models based on the Maximum Mean Discrepancy (MMD) distance.

The use of the MMD distance based on bounded kernels for robust minimum distance estimation was proposed in Barp et al. (2019) and in Chérief-Abdellatif and Alquier (2022) (see also Chérief-Abdellatif and Alquier, 2020, for a Bayesian type estimator).
When unbounded kernels are used the “automatic” robustness induced by the MMD metric is lost, in which case Lerasle et al. (2019) propose a Median-of-Mean procedure to robustify the MMD based estimator. However, all these references focus on the simple case where we have a fully parametric model for the distribution of the data.

In this paper, we first extend the MMD based minimum distance approach of Barp et al. (2019); Chérief-Abdellatif and Alquier (2022) to the regression setting. This task is non-trivial, especially in the random design scenario where we have a statistical model only for the distribution of \( Y | X \), and not for the distribution of \( X \). If the distribution \( P_0^X \) of \( X \) is known then the method in the latter two references can be used for robust inference since, in this case, if we have a model \( \{ P_\theta^Y | X, \theta \in \Theta \} \) for the distribution of \( Y | X \) then we have the model \( \{ P_0^X P_\theta^Y | X, \theta \in \Theta \} \) for the distribution of the pair \((X, Y)\). In practice, \( P_0^X \) is generally unknown but we can use the observations \( \{ X_i \}_{i=1}^n \) to compute an empirical estimate \( \hat{P}_n^X \) of this distribution. In this work, we consider the natural ideal of using \( \{ P_n^X P_\theta^Y | X, \theta \in \Theta \} \) as the model for the distribution of \((X, Y)\) and then to estimate \( \theta \) using the approach introduced in Barp et al. (2019); Chérief-Abdellatif and Alquier (2022). As shown below, it turns out that replacing \( P_0^X \) by the non-parametric estimator \( \hat{P}_n^X \) preserves the convergence and robustness properties of the estimator.

More precisely, we prove that the resulting estimator \( \hat{\theta}_n \) of the model parameter is, in the fixed and random design setting, (i) universally consistent, in the sense that it will always converge to the best approximation, in the sense of the MMD distance, of the truth in the model without any assumption on the distribution generating the observations, and (ii) robust to adversarial contaminations. As a by-product of our theoretical analysis of \( \hat{\theta}_n \) in the random design setting we derive results on kernel conditional mean embedding of distributions that are of independent interest.

Computing \( \hat{\theta}_n \) requires to optimize a function involving a sum over \( n^2 \) terms. We introduce a stochastic gradient algorithm which allows to efficiently compute this estimator from several thousands data points, but the use of \( \hat{\theta}_n \) remains computationally expensive for large datasets. For this reason, we introduce an alternative estimator \( \tilde{\theta}_n \) which, as argued below, is expected to have a similar behaviour to \( \hat{\theta}_n \) in practice while having the advantage to be defined by an objective function involving only a sum over \( n \) terms. We also establish that this estimator is itself robust to outliers, in the sense that its influence function is bounded.

Throughout this work \( \mathcal{X} \) and \( \mathcal{Y} \) are two topological spaces, equipped respectively with the Borel \( \sigma \)-algebra \( \mathcal{G}_\mathcal{X} \) and \( \mathcal{G}_\mathcal{Y} \), and, letting \( \mathcal{Z} = \mathcal{X} \times \mathcal{Y} \) and \( \mathcal{G}_\mathcal{Z} = \mathcal{G}_\mathcal{X} \otimes \mathcal{G}_\mathcal{Y} \), we denote by \( \mathcal{P}(\mathcal{Z}) \) the set of probability distributions on \((\mathcal{Z}, \mathcal{G}_\mathcal{Z})\). We assume below that any distribution \( P \in \mathcal{P}(\mathcal{Z}) \) for \((X, Y)\) admits a regular conditional probability for the distribution of \( Y \) given \( X \) and that all the random variables are defined on the same probability space \((\Omega, \mathcal{F}, \mathbb{P})\).

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1This is for instance the case if \( \mathcal{X} \) and \( \mathcal{Y} \) are two Polish spaces.
2. Kernel mean embedding of distributions: Background and new results

2.1. Notation and convention

We let \( k : \mathbb{Z}^2 \rightarrow \mathbb{R} \) be a kernel on \( \mathcal{Z} \), i.e. \( k \) is symmetric and positive definite, and denote by \((\mathcal{H}, < \cdot, \cdot>_\mathcal{H})\) the reproducing kernel Hilbert space (RKHS) over \( \mathcal{Z} \) having \( k \) as reproducing kernel (see Muandet et al., 2017, for a comprehensive introduction to RKHSs). In addition, we let \( k_\mathcal{X} \) be a kernel on \( \mathcal{X} \), \( k_\mathcal{Y} \) be a kernel on \( \mathcal{Y} \) and denote by \((\mathcal{H}_\mathcal{X}, < \cdot, \cdot>_{\mathcal{H}_\mathcal{X}})\) and by \((\mathcal{H}_\mathcal{Y}, < \cdot, \cdot>_{\mathcal{H}_\mathcal{Y}})\) the RKHS induced by \( k_\mathcal{X} \) and by \( k_\mathcal{Y} \), respectively. When there is no ambiguity, with a slight abuse of language we will refer to \( \mathcal{H} \) as the RKHS on \( \mathcal{Z} \) induced by \( k \), although the full characterization of an RKHS requires to specify both a function space and an inner product. The same abuse of language will be used for the RKHSs induced by \( k_\mathcal{X} \) and by \( k_\mathcal{Y} \). In the following we denote by \( k_\mathcal{X} \otimes k_\mathcal{Y} \) the product kernel on \( \mathcal{Z} \) such that \( k_\mathcal{X} \otimes k_\mathcal{Y}\{ (x, y), (x', y') \} = k_\mathcal{X}(x, x')k_\mathcal{Y}(y, y') \) for all \((x, y), (x', y') \in \mathcal{Z} \), and by \( K_{\alpha, \gamma} \) the Matérn kernel on \( \mathbb{R}^d \) with bandwidth parameter \( \gamma > 0 \) and smoothness parameter \( \alpha \in (0, \infty) \).

We refer to Example 2.2 in Kanagawa et al. (2018) for the general definition \( K_{\alpha, \gamma} \) but we mention here a few useful properties of this kernel. Firstly, \( K_{\alpha, \gamma} \) reduces to the exponential kernel when \( \alpha = 1/2 \), i.e. \( K_{1/2, \gamma}(x, x') = \exp(-||x - x'||/\gamma) \), and to the Gaussian kernel when \( \alpha = \infty \), i.e. \( K_{\infty, \gamma}(x, x') = \exp(-||x - x'||^2/\gamma) \). Secondly, for all \( \alpha \in (0, \infty) \) there exists a function \( \tilde{K}_\alpha : [0, \infty) \rightarrow \mathbb{R} \) such that \( K_{\alpha, \gamma}(x, x') = \tilde{K}_\alpha(||x - x'||/\gamma) \) for all \((x, x') \in \mathbb{R}^2 \) and all \( \gamma > 0 \), implying that the Matérn kernel is a translation invariant kernel. Lastly, for all \( \alpha \in (0, \infty) \) and \( \gamma > 0 \) the Matérn kernel is bounded and continuous.

2.2. Kernel mean embeddings and the maximum mean discrepancy metric

Assume that the following condition on \( k \) holds:

**Assumption A1.** The kernel \( k \) is \( \mathcal{G}_Z \)-measurable and such that \( |k| \leq 1 \).

Then, for any probability distribution \( P \in \mathcal{P}(\mathcal{Z}) \), the quantity \( \mu(P) := E_{Z \sim P}[k(Z, \cdot)] \), called the mean embedding of \( P \), is well defined in \( \mathcal{H} \). If in addition \( k \) is such that the mapping \( P \mapsto \mu(P) \) is one-to-one, in which case \( k \) is said to be characteristic, the mapping \( \mathbb{D}_k : \mathcal{P}(\mathcal{Z})^2 \rightarrow [0, 2] \) defined by

\[
\mathbb{D}_k(P, Q) = ||\mu(P) - \mu(Q)||_{\mathcal{H}}, \quad P, Q \in \mathcal{P}(\mathcal{Z})^2,
\]

is a metric on \( \mathcal{P}(\mathcal{Z}) \), known as the maximum mean discrepancy metric. We stress that none of the results presented in this work requires \( k \) to be characteristic but it is only under this assumption on \( k \) that they provide useful and interpretable convergence guarantees for the proposed estimators.

To better understand the properties of the MMD distance it is useful to express it as an integral probability metric as follows (see, e.g. Muandet et al., 2017)

\[
\mathbb{D}_k(P, Q) = \sup_{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1} \left| E_{Z \sim P}[f(Z)] - E_{Z \sim Q}[f(Z)] \right|, \quad P, Q \in \mathcal{P}(\mathcal{Z})^2.
\]
Two distributions $P$ and $Q$ are therefore close to each other in the sense of the MMD distance if $\mathbb{E}_{Z \sim P}\{f(Z)\} \approx \mathbb{E}_{Z \sim Q}\{f(Z)\}$ for all functions $f \in \mathcal{H}$ with norm at most 1. Both the norm and the set $\mathcal{H}$ depends on $k$ but, under Assumption A1 and if $k$ is characteristic, $\mathcal{H}$ is dense in $C_b(\mathcal{Z})$. In the special case where $\mathcal{Z} \subseteq \mathbb{R}^{d_z}$ for some $d_z \in \mathbb{N}$ and $k$ is characteristic and translation invariant, $\mathbb{D}_k(P,Q)$ is the distance in $L_2(\mathbb{R}^d, \eta_k)$ between the characteristic functions of $P$ and $Q$, for some probability measure $\eta_k \in \mathcal{P}(\mathbb{R}^{d_z})$. For instance, $\eta_k$ is a Gaussian distribution if $k$ is a Gaussian kernel and is a Cauchy distribution if $k$ is an exponential kernel. We refer to Table 2.1 of Muandet et al. (2017) for the expression of $\eta_k$ for various popular translation invariant kernels.

The rest of this section is relevant only for Section 4.3 and can be skipped in a first reading.

### 2.3. Kernel conditional mean embeddings

In the rest of this section we let $(P_{Y|X})_{x \in \mathcal{X}}$ be a collection of distributions on $(\mathcal{X}, \mathcal{G}_\mathcal{X})$, $P_X \in \mathcal{P}(\mathcal{X})$ and $P = P_X P_{Y|X} \in \mathcal{P}(\mathcal{Z})$. In addition, we assume that the following assumption on $k$ holds:

**Assumption A2.** $k = k_X \otimes k_Y$ where $k_X$ and $k_Y$ are continuous on $\mathcal{X}^2$ and on $\mathcal{Y}^2$, respectively, and such that $|k_X| \leq 1$ and $|k_Y| \leq 1$.

This assumption imposes that $\mathcal{H} = \mathcal{H}_X \otimes \mathcal{H}_Y$ and we note that the kernel $k$ is characteristic if $k_X$ and $k_Y$ have the additional properties to be translation invariant and characteristic (Szabó and Sriperumbudur, 2018). Under Assumptions A1-A2 we can define a conditional mean embedding operator of $P$. Such an operator is a mapping $C_{Y|X} : \mathcal{H}_X \rightarrow \mathcal{H}_Y$ such that

$$C_{Y|X} k_X(x, \cdot) = \mu(P_{Y|X}), \quad \forall x \in \mathcal{X}. \quad (1)$$

Since $\mathbb{I}$ depends on $P$ only through $(P_{Y|X})_{x \in \mathcal{X}}$ in what follows we will often refer to $C_{Y|X}$ as the conditional mean embedding operator of $(P_{Y|X})_{x \in \mathcal{X}}$.

A valid definition of a conditional mean embedding operator was only recently proposed by Klebanov et al. (2020), see also Mollenhauer and Koltai (2020); Li et al. (2022), and is expressed in term of the uncentred covariance operator $C_P : \mathcal{H}_X \rightarrow \mathcal{H}_Y$ and in term of the uncentred cross-covariance operator $C_{P_X} : \mathcal{H}_X \rightarrow \mathcal{H}_X$, which are such that, for all $f_1, f_2 \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$,

$$\langle g, C_P f_1 \rangle_{\mathcal{H}_Y} = \mathbb{E}_{(X,Y) \sim P}\{g(Y)f_1(X)\}, \quad \langle f_1, C_{P_X} f_2 \rangle_{\mathcal{H}_X} = \mathbb{E}_{X \sim P_X}\{f_1(X)f_2(X)\}. \quad (2)$$

The boundedness of $k_X$ and $k_Y$, imposed by Assumption A2, implies that $C_P$ and $C_{P_X}$ exist, are unique, and that they are bounded linear operators (see Fukumizu et al., 2004, Section 3).

With this notation in place, we obtain the following slight variation of Klebanov et al. (2020, Theorem 5.3), whose proof is given in the Appendix for sake of completeness.
Lemma 1. Assume that Assumptions A1-A2 hold, that the function \( f \in H_X \) is such that 
\[
\mathbb{E}_{X \sim P_X}\{f^2(X)\} = 0 \quad \text{if and only if} \quad f = 0,
\]
and that 
\[
\mathbb{E}_{Y \sim P_Y}\{g(Y)\} \in H_X, \quad \forall g \in H_Y.
\] (3)

Then, (1) holds for the bounded linear operator \( C_{Y \mid X} = (C_{P_X}^\dagger C_{P_Y}^*)^\ast \), where \( C_{P_X}^\dagger \) denotes the Moore-Penrose pseudo-inverse of \( C_{P_X} \).

In this work, we use the following property of conditional mean embedding operators:

Lemma 2. For \( P'_X, P''_X \in \mathcal{P}(\mathcal{X}) \), let \( P' = P'_X P_{Y \mid} \) and \( P'' = P''_X P_{Y \mid} \), and assume that \( (P_{Y \mid x})_{x \in \mathcal{X}} \) admits a bounded linear conditional mean embedding operator \( C_{Y \mid X} \). Then,

\[
\mathbb{D}_k(P', P'') \leq \|C_{Y \mid X}\|_0 \mathbb{D}_{k^2_X}(P'_X, P''_X).
\] (4)

In words, conditional mean embedding operators allow to quantify the MMD distance between two joint distributions \( P' \) and \( P'' \) on \((Z, S_Z)\), having the same regular conditional distribution \( (P_{Y \mid x})_{x \in \mathcal{X}} \), in term of the MMD distance, induced by the kernel \( k^2_X \), between their marginals \( P'_X \) and \( P''_X \).

2.4. Some clarifications on kernel conditional mean embeddings

The main difficulty of the theory of conditional mean embedding operators is that condition (3), introduced by Song et al. (2009), is hard to interpret. This condition is slightly weakened in Klebanov et al. (2020) but the alternative assumptions proposed in this reference remain hard to interpret since, as in (3), they require that all functions in \( H_Y \) satisfy a given property. In fact, to the best of our knowledge, there is no explicit examples of distributions \( (P_{Y \mid x})_{x \in \mathcal{X}} \) for which a conditional mean embedding operator exists, beyond the trivial case where \( P_{Y \mid x} \) does not depend on \( x \). Below, we fill this important gap assuming that, for all \( x \in \mathcal{X} \), the distribution \( P_{Y \mid x} \) is dominated by some \( \sigma \)-finite measure \( \mu(dy) \).

We start by stating a theorem that provides sufficient conditions for (3) to hold which only involve the Radon-Nikodym derivatives of \((P_{Y \mid x})_{x \in \mathcal{X}}\) w.r.t. \( \mu(dy) \).

Theorem 1. Assume that Assumptions A1-A2 hold and that there exists a \( \sigma \)-finite measure \( \mu(dy) \) on \((\mathcal{Y}, S_Y)\) such that \( P_{Y \mid x} = p(y \mid x) \mu(dy) \) for all \( x \in \mathcal{X} \), where \( p(\cdot \mid x) \) is such that the following conditions hold:

1. We have \( p(y \mid x) \in H_X \) for all \( y \in \mathcal{Y} \).
2. The function \( \mathcal{Y} \ni y \mapsto p(y \mid x) \) is Borel measurable.
3. For all \( y' \in \mathcal{Y} \) the set \( \{k_Y(y', y)p(y \mid x), y \in \mathcal{Y}\} \) is separable.
4. We have \( \int_{\mathcal{Y}} \|p(y \mid x)\|_{H_X} \mu(dy) < \infty \).

Then, condition (3) holds.
If \( \mathcal{Y} \) is a finite set then Conditions 2-4 of Theorem 1 always hold while Condition 4 is implied by Condition 1. Hence, in this case, assuming Conditions 1-3 reduces to assuming Condition 1, which is both sufficient and necessary for 4 to hold when \( \mathcal{Y} \) is a finite set. When \( \mathcal{Y} \) is not finite the additional Conditions 2-4 are used to show that, for all \( g \in \mathcal{H}_\mathcal{Y} \), the function \( y \mapsto g(y)p(y|\cdot) \) is Bochner integrable and thus that \( \mathbb{E}_{Y \sim P_Y}\{g(Y)\} \) is a well-defined function on \( \mathcal{X} \).

The conclusions of Lemma 1 and Theorem 1 are summarized in the following result:

**Corollary 1.** Consider the set-up of Theorem 1 and assume that \( f \in \mathcal{H}_X \) is such that \( \mathbb{E}_{X \sim P_X}\{f^2(X)\} = 0 \) if and only if \( f = 0 \). Then, there exists a bounded conditional mean embedding operator \( C_{Y|X} \) for \( (P_{Y|X})_{x \in \mathcal{X}} \) which is such that \( \|C_{Y|X}\|_0 \leq \int_{\mathcal{Y}} \|p(y|\cdot)\|_{\mathcal{H}_X}^2 \mu(dy) \).

In general, RKHS norms are hard to interpret. However, if \( k_X \) is a Matérn kernel and \( \mathcal{X} \subset \mathbb{R}^d \) is a bounded set with Lipschitz boundary, e.g. \( \mathcal{X} \) is a hypercube, then the RKHS \( (\mathcal{H}_X, <\cdot, \cdot>_\mathcal{H}_X) \) is norm equivalent to a Sobolev space (see e.g. [Kanagawa et al., 2018, Example 2.6]). As shown in Appendix E together with Theorem 1 this property of Matérn kernels allows to obtain explicit conditions on the Radon-Nikodym derivatives \( (p(\cdot|x))_{x \in \mathcal{X}} \) of \( (P_{Y|X})_{x \in \mathcal{X}} \) which are sufficient to ensure that, under mild assumptions on \( k_Y \), condition 3 holds. This allows us to establish the following proposition, which provides for various definitions of \( \mathcal{Y} \) non-trivial examples of distributions \( (P_{Y|X})_{x \in \mathcal{X}} \) that admit a bounded conditional mean embedding operator with respect to a characteristic kernel \( k \).

**Proposition 1.** Let \( \mathcal{X} \subset \mathbb{R}^d \) be a bounded set with Lipschitz boundary and strictly positive Lebesgue measure, \( k_\mathcal{X} \) be the restriction of the Matérn kernel \( K_{\frac{d}{2},\gamma} \) on \( \mathcal{X} \times \mathcal{X} \), for some \( m \in \mathbb{N} \) and \( \gamma > 0 \), and let \( k_Y \) be a continuous, translation invariant, bounded and characteristic kernel on \( \mathcal{Y} \). Then, \( k = k_\mathcal{X} \times k_Y \) is characteristic and there exists a bounded conditional mean embedding operator for \( (P_{Y|X})_{x \in \mathcal{X}} \) when, for all \( x \in \mathcal{X} \),

- \( P_{Y|x} = \sum_{m=1}^M w_m N(\beta_m^T x, \sigma_m^2) \) for some \( M \in \mathbb{N} \), non-negative real numbers \( \{w_m\}_{m=1}^M \) such that \( \sum_{m=1}^M w_m = 1 \), vectors \( \{\beta_m\}_{m=1}^M \) in \( \mathbb{R}^d \) and strictly positive real numbers \( \{\sigma_m\}_{m=1}^M \), so that \( \mathcal{Y} = \mathbb{R} \).
- \( P_{Y|x} = \text{Pois}\{\exp(\beta^T x)\} \) for some \( \beta \in \mathbb{R}^d \), so that \( \mathcal{Y} = \mathbb{N}_0 \).
- \( P_{Y|x} = \text{Ber}[1/\{1 + \exp(\beta^T x)\}] \) for some \( \beta \in \mathbb{R}^d \), so that \( \mathcal{Y} = \{0, 1\} \).
- \( P_{Y|x} = \text{Gamma}\{\nu, \nu \exp(-\beta^T x)\} \) for some \( \beta \in \mathbb{R}^d \) and \( \nu \in (0, \infty) \), so that \( \mathcal{Y} = (0, \infty) \).
- \( P_{Y|x} \) is the distribution of \((Y_{x,1}, Y_{x,2})\), where \( Y_{x,2} = \mathbb{I}_{(0,\infty)}(Y_{x,2}^*) \) and \( Y_{x,1} = Y_{x,2}Y_{x,1}^* \) with

\[
\begin{pmatrix} Y_{x,1}^* \\ Y_{x,2}^* \end{pmatrix} \sim \mathcal{N}_2\left( \begin{pmatrix} \beta^T x \\ \gamma^T x \end{pmatrix}, \begin{pmatrix} \sigma^2 & \rho \sigma \\ \rho \sigma & 1 \end{pmatrix} \right)
\]

for some \( \beta, \gamma \in \mathbb{R}^d \), \( \sigma > 0 \) and \( \rho \in (-1, 1) \), so that \( \mathcal{Y} = \mathbb{R} \times \{0, 1\} \).
The above assumptions on \( k_Y \) are satisfied if \( k_Y \) is the restriction on \( \mathcal{Y} \times \mathcal{Y} \) of a Matérn kernel on \( \mathbb{R}^d_Y \), with \( d_y = 1 \) for the first four definitions of \( (P_{Y|x})_{x \in \mathcal{X}} \) and with \( d_y = 2 \) for the last one.

**Remark 1.** The assumptions on \( \mathcal{X} \) are satisfied e.g. when this set is a non-empty open-hypercube.

### 3. MMD-based regression

#### 3.1. Set-up

We let \( \{P_{\lambda}, \lambda \in \Lambda\} \) be a set of probability distributions on \((\mathcal{Y}, \mathcal{G}_Y)\), \( \Theta \) be a Polish space and \( g : \Theta \times \mathcal{X} \to \Lambda \) be such that the mapping \( x \mapsto P_{g(\theta,x)}(A) \) is \( \mathcal{G}_X \)-measurable for all \( A \in \mathcal{G}_Y \) and all \( \theta \in \Theta \). Then, given a \( Z \)-valued random variable \((X,Y)\), with \( Y \) taking values in \( \mathcal{Y} \), we consider the statistical model \( \{(P_{g(\theta,x)})_{x \in \mathcal{X}}, \theta \in \Theta\} \) for the conditional distribution of \( Y \) given \( X \). For example, the Gaussian linear regression model with known variance is obtained by taking \( P_{\lambda} = N_1(\lambda, \sigma^2) \) and \( g(\theta, x) = \theta \top x \), the logistic regression model by taking \( P_{\lambda} = \text{Ber}(\lambda) \) and \( g(\theta, x) = 1/(1 + \exp(-\theta \top x)) \), and the Poisson regression model by taking \( P_{\lambda} = \text{Pois}(\lambda) \) and \( g(\theta, x) = \exp(\theta \top x) \). Other classical examples include binomial, exponential, gamma and inverse-Gaussian regression models.

In the following, \( k \) is a kernel on \( Z \) satisfying Assumption [A1] stated in Section 2, and \( D_n = \{(X_i, Y_i)\}_{i=1}^n \) is a set of \( n \) random variables taking values in \( Z \). Below we assume that a realization of \( D_n \) is used to fit the regression model \( \{(P_{g(\theta,x)})_{x \in \mathcal{X}}, \theta \in \Theta\} \) and, for this reason, we will often refer to \( D_n \) as the observations.

#### 3.2. Definition of the estimators \( \hat{\theta}_n \) and \( \tilde{\theta}_n \)

Let \( \hat{P}^n = (1/n) \sum_{i=1}^n \delta_{(X_i, Y_i)} \) be the empirical distribution of the observations and, for every \( \theta \in \Theta \), let \( \hat{P}^n_{\theta} \) be the (random) probability distribution on \((Z, \mathcal{G}_Z)\) defined by

\[
\hat{P}^n_{\theta}(A \times B) = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}(A) P_{g(\theta,X_i)}(B), \quad A \times B \in \mathcal{G}_X \otimes \mathcal{G}_Y. \tag{5}
\]

In other words, if \((X,Y) \sim \hat{P}^n_{\theta} \) then \( X \) is uniformly distributed on the set \( \{X_1, \ldots, X_n\} \) and \( Y|(X = x) \sim P_{g(\theta,x)} \).

The first estimator introduced in this work, \( \hat{\theta}_n \), is defined through the minimization of the MMD between the probability distributions \( \hat{P}^m_{\theta} \) and \( \hat{P}^n \), that is

\[
\hat{\theta}_n(D_n) \in \arg\min_{\theta \in \Theta} \mathbb{D}^2_k(\hat{P}^m_{\theta}, \hat{P}^n) = \arg\min_{\theta \in \Theta} \hat{F}_n(\theta), \quad \hat{F}_n(\theta) := \sum_{i,j=1}^n \hat{\ell}(\theta, X_i, X_j, Y_j) \tag{6}
\]

\(^2\text{When such a minimizer does not exist, we can use an \( \epsilon \)-minimizer instead and that follows can be trivially adapted. In addition, we implicitly assume that \( \theta_n \) and \( \hat{\theta}_n \) are measurable, for all } n \geq 1.\)
where, for all $\theta \in \Theta$, $(x, x') \in \mathcal{X}^2$ and $y \in \mathcal{Y}$,

$$
\hat{\ell}(\theta, x, x', y) = \mathbb{E}_{Y \sim P(y_{\theta,x}), Y' \sim P(y_{\theta,x'})} \left\{ k \{ (x, Y), (x', Y') \} - 2k \{ (x, Y), (x', y) \} \right\}.
$$

(7)

Under Assumption A1, the kernel $k$ is bounded so that each term in the double sum appearing in the definition of $\hat{F}_n$ is bounded by 3. Intuitively, this limits the impact that a single observation can have on $\hat{\theta}_n(D_n)$, making this estimator robust to outliers.

The number of terms in the definition of the function $\hat{F}_n$ to minimize is $\mathcal{O}(n^2)$. Below we propose an approach that makes possible to efficiently compute $\hat{\theta}_n$ for moderate values of $n$, that is for $n$ equals to a few thousands, but this feature of $\hat{F}_n$ limits the applicability of $\hat{\theta}_n$ in large datasets. For large scale problems we propose the alternative estimator $\tilde{\theta}_n$, defined by

$$
\tilde{\theta}_n(D_n) \in \arg\min_{\theta \in \Theta} \hat{F}_n(\theta), \quad \hat{F}_n(\theta) := \sum_{i=1}^{n} \hat{\ell}(\theta, X_i, Y_i)
$$

(8)

where, for all $\theta \in \Theta$, $x \in \mathcal{X}$ and $y \in \mathcal{Y}$,

$$
\hat{\ell}(\theta, x, y) = \mathbb{E}_{Y, Y' \sim P(y_{\theta,x})} \left\{ k_Y(Y, Y') - 2k_Y(Y, y) \right\}.
$$

(9)

The function $\hat{F}_n$ defined in (8) has the advantage to involve only $n$ terms but, on the other hand, $\hat{\theta}_n$ cannot be interpreted as the minimizer of a measure of discrepancy between $\hat{P}^n_{\theta}$ and $P^n$. Theoretical results regarding the robustness properties of $\hat{\theta}_n$ are provided in the next section, they are weaker than those obtained for $\tilde{\theta}_n$.

Henceforth we use the shorthand $\hat{\theta}_n = \hat{\theta}_n(D_n)$ and $\tilde{\theta}_n = \tilde{\theta}_n(D_n)$, which is standard in statistics.

### 3.3. Link between the two estimators

In this subsection we assume that $k = k_{\mathcal{X}} \otimes k_{\mathcal{Y}}$ where $k_{\mathcal{X}} = k_{\gamma}$ for some kernel $k_{\gamma}$ on $\mathcal{X}$ such that $k_{\gamma}(x, x) = 1$ and such that $\lim_{x' \to x} k_{\gamma}(x, x') = 0$ for all $x' \neq x$. When $\mathcal{X} \subseteq \mathbb{R}^d$ these two properties are for instance satisfied when, for some $\alpha \in (0, \infty)$, the kernel $k_{\gamma}$ is a Matérn kernel, that is when $k_{\gamma} = K_{\gamma}$ with $K_{\gamma}$ as introduced in Section 2.1.

Let $\ell(\theta, x, x', y) = \hat{\ell}(\theta, x, x', y)/k_{\gamma}(x, x')$ if $k_{\gamma}(x, x') \neq 0$ and $\ell(\theta, x, x', y) = 0$ otherwise. Under the above assumptions on $k$ the quantity $\ell(\theta, x, x', y)$ does not depend on $k_{\gamma}$ and is such that $\ell(\theta, x, x, y) = \hat{\ell}(\theta, x, y)$. Therefore, letting

$$
h_n(\gamma, \theta, D_n) = 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} k_{\gamma}(X_i, X_j) \ell(\theta, X_i, X_j, Y),
$$

(10)

it follows that the estimators $\hat{\theta}_n$ and $\tilde{\theta}_n$ are such that

$$
\hat{\theta}_n \in \arg\min_{\theta \in \Theta} \left\{ \sum_{i=1}^{n} \ell(\theta, X_i, Y_i) + h_n(\gamma, \theta, D_n) \right\}, \quad \tilde{\theta}_n \in \arg\min_{\theta \in \Theta} \sum_{i=1}^{n} \ell(\theta, X_i, Y_i).
$$
Consequently, using \( \hat{\theta}_n \) in place of \( \hat{\theta}_n \) amounts to discarding, in the definition of this latter estimator, the term \( h_n(\gamma, \theta, D_n) \) whose computation requires \( O(n^2) \) operations. Assuming that the \( X_i \)'s are \( P \)-a.s. distinct, under the above assumptions on \( k_n \) for all \( \theta \in \Theta \) we have \( \lim_{n \to 0} h_n(\gamma, \theta, D_n) = 0 \), \( P \)-a.s. Therefore, under suitable continuity assumptions, \( \hat{\theta}_n \to \hat{\theta}_n \) as \( \gamma \to 0 \), \( P \)-a.s. For this reason, and as illustrated in Section 4 for a small value of \( \gamma \) we expect the two estimators \( \hat{\theta}_n \) and \( \hat{\theta}_n \) to have a very similar behaviour in practice.

3.4. Computation of the two estimators

Computing the estimators \( \hat{\theta}_n \) and \( \hat{\theta}_n \) require optimizing the functions \( \bar{F}_n \) and \( \tilde{F}_n \), respectively, which are both defined through an expectation. In some models the expectations appearing in (7) and in (9) can be computed explicitly, in which case the functions \( \tilde{F}_n \) and \( \bar{F}_n \) has a known expression and standard optimization algorithms can be used to optimize them. This is for example the case in logistic or multinomial regression, since for these two models the expectations in (7) and in (9) are finite sums.

In general, the functions \( \tilde{F}_n \) and \( \bar{F}_n \) are however intractable, and as a general strategy for computing \( \hat{\theta}_n \) and \( \hat{\theta}_n \) we propose the use of a stochastic gradient algorithm. As shown in Appendix A.1 under suitable regularity conditions we have

\[
\nabla_{\theta} \ell(\theta, x, x', y) = 2E_{Y \sim P_{g(\theta, x), Y' \sim P_{g(\theta, x')}} \left[ k\{(x, Y), (x', Y')\} - k\{(x, Y), (x', y)\}\right]\nabla_{\theta} \log p_{g(\theta, x)}(Y)
\]

and

\[
\nabla_{\theta} \tilde{\ell}(\theta, x, y) = 2E_{Y, Y' \sim P_{g(\theta, x)}} \left[ \{k y(Y, Y') - k y(Y, y)\}\right]\nabla_{\theta} \log p_{g(\theta, x)}(Y)
\]

so that we can easily compute an unbiased estimate of \( \nabla \tilde{F}_n(\theta) \) and of \( \nabla \bar{F}_n(\theta) \) under the mild conditions that (i) we can sample from \( P_\lambda \) for all \( \lambda \in \Lambda \) and (ii) that we can compute the gradient of the log-likelihood function of a single observation. The stability of this procedure obviously depends on the model, but it holds generally at least for compact parameter spaces \( \Theta \), as discussed in Appendix A.1.

It is important to stress that the functions \( \tilde{F}_n \) and \( \bar{F}_n \), being typically non-convex and potentially multi-modal, notably in the presence of outliers, the starting value of the stochastic gradient algorithm must be chosen with care. When the maximum likelihood estimator of the model parameter can be efficiently computed we recommend to use its value to initialize the optimization procedure. Otherwise, the gradient-free algorithm introduced in Gerber and Douc (2022), designed to compute the global optimum of a function defined through an expectation, can be used to find a good starting value for the stochastic gradient algorithm.

It is important to mention at this stage that the computation of \( \hat{\theta}_n \) can be greatly facilitated by taking \( k = k_X \otimes k_Y \) where \( k_X = k_\gamma \) with \( k_\gamma \) as in Section 3.3. Indeed, for such a kernel \( k \) it often true that with high probability we have \( k_\gamma(X_i, X_j) \approx 0 \) for all \( i \neq j \), and thus that \( h_n(\gamma, \theta, D_n) \approx 0 \), where \( h_n(\gamma, \theta, D_n) \) is as defined in (10). In this case, we can efficiently compute \( \hat{\theta}_n \) with a stochastic gradient algorithm whose cost per iteration is linear in the sample size \( n \), as explained in Appendix A.2.
4. Theoretical analysis

4.1. Set-up and summary of the main results

In this section we introduce theoretical results concerning the robustness of the estimators \( \hat{\theta}_n \) and \( \tilde{\theta}_n \) when outliers are present in the dataset used by the statistician to fit the regression model. To this aim, we need to interpret \( D_n \) as a contaminated version of a dataset \( D^0_n := \{(X^0_i, Y^0_i)\}_{i=1}^n \), and below we consider two contamination models, namely the Huber contamination model (Huber, 1992) and the adversarial contamination model, defined in Definition 1 and in Definition 2 respectively.

**Definition 1.** We say that the observed dataset \( D_n \) is an \( \epsilon \)-adversarial contamination of \( D^0_n \) if there exists a set \( I \subset \{1, \ldots, n\} \) such that \( |I|/n \leq \epsilon \) and such that \( (X_i, Y_i) = (X^0_i, Y^0_i) \) for all \( i \notin I \).

**Definition 2.** We say that the observed dataset \( D_n \) is an \((\epsilon, Q)\)-Huber contamination of \( D^0_n \) if there exists a \( Q \in \mathcal{P}(\mathbb{Z}) \) such that \( (X_i, Y_i) \sim \epsilon Q + (1 - \epsilon) \delta_{(X^0_i, Y^0_i)} \) for all \( i \in \{1, \ldots, n\} \).

Below we derive non-asymptotic bounds for \( \hat{\theta}_n \) under both the fixed design and the random design scenarios, which prove the robustness of this estimator to adversarial contaminations of the data. For \( \tilde{\theta}_n \) we derive an asymptotic result in the random design case which establishes the robustness of this estimator to Huber contaminations of the sample.

Recall that results in the fixed design case only provide guarantees on the estimation of the distribution of \( Y \) when \( X \) is equal to one of the observed \( X_i \)'s, while in practice regression is often used for out-of-sample predictions. In this case, and assuming that the pairs \( (Y^0_i, X^0_i) \)'s are i.i.d, this means that we want guarantees on the estimation of the distribution of \( Y \) when \( X \) is drawn from the same, unknown, distribution as the observed \( X_i \)'s, and independently from them. This is precisely what theoretical results in the random design case provide.

In what follows we let \( P^0_{Y|x} \) be a regular conditional probability of \( Y \) given \( X \), and thus \( Y^0_i |(X^0_i = x) \sim P^0_{Y|x} \) for all \( x \in \mathcal{X} \) and all \( i = 1, \ldots, n \).

4.2. Non-asymptotic bounds for the estimator \( \hat{\theta}_n \)-- Fixed design

A typical scenario for the fixed design case is when the \( X^0_i \)'s are experimental settings that are carefully planned in advance. In this case, measurement errors can only affect the \( Y^0_i \)'s. For this reason, in this subsection we assume that the contamination of the sample occurs only on the \( Y^0_i \)'s, so that \( X_i = X^0_i \) for all \( i \in \{1, \ldots, n\} \).

Letting

\[
\hat{P}^0_n(A \times B) = \frac{1}{n} \sum_{i=1}^n \delta_{X^0_i}(A)P^0_{Y|X^0_i}(B), \quad \forall (A \times B) \in \mathcal{G}_Z,
\]

we set up our objective as the reconstruction of \( \hat{P}^0_n \in \mathcal{P}(\mathbb{Z}) \) by a distribution in the set \( \{\hat{P}^0_n, \theta \in \Theta\} \).
The following lemma gives a non-asymptotic bound on the performances of the estimator \( \hat{\theta}_n \) for this task, under an adversarial contamination of the sample.

**Lemma 3.** Assume that \( D_n \) is an \( \epsilon \)-adversarial contamination of \( D_0^n \) such that \( X_i = X_0^i \) for all \( i \in \{1, \ldots, n\} \). Then, under Assumption [A1]

\[
\mathbb{E}\{D_k(\hat{P}^n_{\hat{\theta}_n}, \bar{P}_0^n)\} \leq 4\epsilon + \inf_{\theta \in \Theta} D_k(\hat{P}_\theta^n, \bar{P}_0^n) + 2/\sqrt{n}
\]

and, for all \( \eta \in (0,1) \),

\[
P\left[D_k(\hat{P}^n_{\hat{\theta}_n}, \bar{P}_n^n) < 4\epsilon + \inf_{\theta \in \Theta} D_k(\hat{P}_\theta^n, \bar{P}_0^n) + n^{-1/2}\{2 + 2\log(1/\eta)\}\right] \geq 1 - \eta. \tag{11}
\]

**Remark 2.** Lemma 3 does not require any assumption on the distribution of \( \{(X_0^i, Y_0^i)\}_{i=1}^n \).

In statistical theory we often assume that the “truth is in the model”, that is that there is a \( \theta_0 \in \Theta \) such that \( \hat{P}^n_{\theta_0} = \bar{P}_0^n \). In this case, Lemma 3 shows that

\[
\mathbb{E}\{D_k(\hat{P}^n_{\theta_0}, \bar{P}_0^n)\} \leq 4\epsilon + 2/\sqrt{n} \tag{12}
\]

while, in the non-contaminated case where \( D_n = D_0^n \),

\[
\mathbb{E}\{D_k(\hat{P}^n_{\theta_0}, \bar{P}_0^n)\} \leq 2/\sqrt{n}. \tag{13}
\]

In words, when computed from the uncontaminated dataset \( D_0^n \) the estimator \( \hat{\theta}_n \) is consistent for estimating \( \theta_0 \), with respect to the MMD distance, and, provided that \( \epsilon \) is small, an \( \epsilon \)-adversarial contamination of the sample will have only a negligible impact on the estimated parameter value. Similar conclusions can be derived from the inequality in probability given in (11).

Lemma 3 implies the convergence of \( \hat{\theta}_n \) with respect to the MMD distance. However, under additional assumptions, it is possible to relate this form of convergence to the convergence in the sense of the Euclidean distance \( \| \cdot \| \) to the true parameter, or the pseudo-true parameter.

**Theorem 2.** Consider the set-up of Lemma 3 and assume that there is a unique \( \theta_0 \in \Theta \) such that \( D_k(\hat{P}^n_{\theta_0}, \bar{P}_0^n) = \inf_{\theta \in \Theta} D_k(\hat{P}_\theta^n, \bar{P}_0^n) \). In addition, assume that there exist a neighbourhood \( U \) of \( \theta_0 \) and a constant \( \mu > 0 \) such that \( D_k(\hat{P}_\theta^n, \hat{P}^n_{\theta_0}) \geq \mu \| \theta - \theta_0 \| \) for all \( \theta \in U \). Let \( \alpha = \inf_{\theta \in U} D_k(\hat{P}_\theta^n, \hat{P}^n_{\theta_0}) \in (0,2] \) and assume that \( \epsilon \in (0, \alpha/32) \). Then,

\[
P\left(\limsup_{n \to \infty} \| \hat{\theta}_n - \theta_0 \| \leq 4\epsilon/\mu \right) = 1
\]

and, for all \( n \geq 64/\alpha^2 \) and all \( \eta \in [2e^{-n\alpha^2/38}, 1) \),

\[
P\left(\| \hat{\theta}_n - \theta_0 \| < (4\epsilon/\mu) + n^{-1/2}\{2 + \sqrt{2\log(2/\eta)}\}/\mu \right) \geq 1 - \eta.
\]
4.3. Non-asymptotic bounds for the estimator $\hat{\theta}_n$—Random design

We assume now that the pairs $(X_0^i, Y_0^i)$’s are i.i.d. from some probability distribution $P^0 \in \mathcal{P}(Z)$, and we denote by $P^0_X$ the marginal distribution of the $X_0^i$’s. In addition, for every $\theta \in \Theta$ we let $P_\theta \in \mathcal{P}(Z)$ be defined by

$$P_\theta(A \times B) = E_{X \sim P^0_X} \{ 1_{A}(X)P_\theta(\theta,X)(B) \}, \quad A \times B \in \mathcal{G}_Z.$$  

Then, we set up our objective as the reconstruction of $P^0$ by a distribution in $\{P_\theta, \theta \in \Theta\}$, and our natural candidate is $P_{\hat{\theta}_n}$.

Since the approximating set $\{P_\theta, \theta \in \Theta\}$ is unknown, because it depends on $P^0_X$, achieving this objective requires more care than in the fixed design setting. In particular, it requires to control the MMD distance between the distribution $P_\theta$ and its empirical counterpart $\tilde{P}_n$ defined in (13), a task that we perform using Lemma 2. For this reason, the results presented below assume that $k = k_X \otimes k_Y$ and require the following additional assumption:

**Assumption A3.** For all $\theta \in \Theta$ there exists a bounded linear conditional mean embedding operator $C_\theta : \mathcal{H}_X \rightarrow \mathcal{H}_Y$ for $(P_\theta(x,x))_{x \in \mathcal{X}}$. In addition, $\mathcal{C} := \sup_{\theta \in \Theta} \|C_\theta\|_0 < \infty$.

Under this additional assumption we have the following result:

**Lemma 4.** Assume that $D_n$ is an $\epsilon$-adversarial contamination of $D_n^0$. Then, under Assumptions A1-A3 and with $\mathcal{C} < \infty$ as in Assumption A3, we have

$$E\{ \mathbb{D}_k(P_{\hat{\theta}_n}, P^0) \} \leq 8\epsilon + \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) + (\mathcal{C} + 3)/\sqrt{n}$$

and, for all $\eta \in (0,1)$,

$$P\left[ \mathbb{D}_k(P_{\hat{\theta}_n}, P^0) < 8\epsilon + \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) + n^{-1/2}(\mathcal{C} + 3)\left\{ 1 + \sqrt{2\log(4/\eta)} \right\} \right] \geq 1 - \eta.$$

From Lemma 4 we can readily obtain the random design counterpart of the inequalities (12)-(13), obtained in the fixed design setting, to prove the consistency of $\hat{\theta}_n$ in the well-specified case and in the absence of contamination.

The following theorem is the main result of this subsection.

**Theorem 3.** Assume that there is a unique $\theta_0 \in \Theta$ such that $\mathbb{D}_k(P_0, P^0) = \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0)$ and that there exist a neighbourhood $U$ of $\theta_0$ and a constant $\mu > 0$ such that

$$\mathbb{D}_k(P_\theta, P^0) \geq \mathbb{D}_k(P_0, P^0) + \mu \|\theta - \theta_0\|, \quad \forall \theta \in U.$$  

(14)

Let $\alpha = \inf_{\theta \in U} \mathbb{D}_k(P_\theta, P^0) - \mathbb{D}_k(P_0, P^0) \in (0,2]$ and assume that $D_n$ is an $\epsilon$-adversarial contamination of $D_n^0$ for some $\epsilon \in [0, \alpha/64]$. Assume also that Assumptions A1-A3 hold and let $\mathcal{C} < \infty$ be as in Assumption A3. Then,

$$P\left( \limsup_{n \rightarrow \infty} \|\hat{\theta}_n - \theta_0\| \leq 8\epsilon/\mu \right) = 1$$

and there exist constants $C_1, C_2 \in (0,\infty)^2$, that depend only on $\alpha$ and on $\mathcal{C}$, such that for all $n \geq C_1$ and all $\eta \in [\epsilon^{-C_2n},1)$ we have

$$P\left[ \|\hat{\theta}_n - \theta_0\| < (8\epsilon/\mu) + n^{-1/2}(\mathcal{C} + 3)\left\{ 1 + \sqrt{2\log(8/\eta)} \right\}/\mu \right] \geq 1 - \eta.$$
Remark 3. If $P^0 = P_{\theta_0}$ for some $\theta_0 \in \Theta$, i.e. if the model is well-specified, then a sufficient condition for $\theta_0$ to be the unique global minimizer of the mapping $\theta \mapsto \mathbb{D}_k(\theta, P^0)$ is that $k$ is characteristic and the model $\{P_{\theta}, \theta \in \Theta\}$ is identifiable, in the sense that $\theta_1 \neq \theta_2 \Rightarrow P_{\theta_1} \neq P_{\theta_2}$.

In Theorem 1 the distribution $P_{\theta_0}$ should be interpreted as the best approximation of $P^0$ in the sense of the MMD distance $\mathbb{D}_k$. It is well-specified, in which case $P_{\theta_0} = P^0$, both the parameter value $\theta_0$ and the distribution $P_{\theta_0}$ depend on the choice of $k$. If a small fraction $\epsilon$ of the data is corrupted then the theorem ensures that $\hat{\theta}_n$ still estimates well $\theta_0$. In particular, the first part of Theorem 1 implies that the influence function of the estimator $\hat{\theta}_n$ is bounded. It is also worth noting that taking $\epsilon = 0$ in Theorem 1 establishes the almost sure convergence of $\hat{\theta}_n$ towards $\theta_0$.

Condition (14) of Theorem 1 requires that the function $\theta \mapsto \mathbb{D}_k(\theta, P^0) = \mathbb{D}_k(P_{\theta_0}, P^0)$ is strongly convex in a neighbourhood $U$ of $\theta_0$, a condition which is rather weak, as shown in the next proposition.

Proposition 2. Assume that $\theta_0 \in \text{argmin}_{\theta \in \Theta} \mathbb{D}_k(\theta, P^0)$ is unique and that the function $\theta \mapsto \mathbb{D}_k(\theta, P^0)$ is twice continuously differentiable at $\theta_0$. Then, condition (14) of Theorem 1 holds.

Proposition 1, given in Section 2.3, provides examples of characteristic kernels $k$ for which, for all $\theta \in \Theta$, a conditional mean embedding operator $C_\theta$ of $(P_{g(\theta,x)})_{x \in \mathcal{X}}$ exists for five popular regression models, namely for (i) the linear Gaussian regression model, first example of Proposition 1 with $\theta = (\beta, \sigma)$, as well as for mixtures of such models, (ii) the Poisson regression model, second example of Proposition 1 with $\theta = \beta$, (iii) the logistic regression model, third example of Proposition 1 with $\theta = \beta$, (iv) the Gamma regression model, fourth example of Proposition 1 with $\theta = (\beta, \nu)$, and (v) the Heckman sample selection model, last example of Proposition 1 with $\theta = (\beta, \gamma, \sigma, \rho)$.

Using the last part of Corollary 1, one can easily check that for each of these models, under a suitable definition of $\Theta$ we have $\sup_{\theta \in \Theta} \|C_\theta\|_a < \infty$, as required by Assumption A3. In the set-up of Proposition 1 this is for instance the case if, for some compact set $B \subset \mathbb{R}^d$ and some $\delta > 0$, the parameter space $\Theta$ is such that $\beta \in B$ for all models, such that $\gamma \in B$ for the Heckman sample selection model, such that $\sigma > \delta$ for the linear Gaussian regression model or mixtures of such models, and for the Heckman sample selection model, such that $\nu \in (\delta, 1/\delta)$ for the Gamma regression model.

Remark 4. Proposition 1 assumes that $\mathcal{X} \subset \mathbb{R}^d$ is a bounded set and, as illustrated with the above examples, Assumption A3 typically holds when $\Theta$ is a compact set. It is however important to note that the dependence to the outliers of the bounds given in Lemma 2 and in Theorem 3 depend neither on $\Theta$ nor on $\mathcal{X}$. Indeed, the outliers impact these bounds only through their proportion $\epsilon$.

4.4. Asymptotic guarantees for the estimator $\hat{\theta}_n$—Random design

For this estimator we set up our objective as the reconstruction of the regular conditional probability $(P^0_{\theta|x})_{x \in \mathcal{X}}$ by a distribution in the set $\{(P_{g(\theta,x)})_{x \in \mathcal{X}}, \theta \in \Theta\}$. As in Section
4.3 In what follows we denote by $P^0$ the distribution of the $(X_i^0, Y_i^0)$’s. In addition, for any distribution $Q \in \mathcal{P}(\mathcal{Z})$ we let $Q_X$ denote the distribution of $X$ and $(Q|_{Y=\cdot})_{x \in \mathcal{X}}$ denote a regular conditional probability for the distribution of $Y$ given $X$, where $(X, Y) \sim Q$.

It is direct to see that $\hat{\theta}_n$ is an $M$-estimator and therefore sufficient conditions on $k_Y$ and on the statistical model to ensure that $\hat{\theta}_n$ converges to some value $\hat{\theta}_0 \in \Theta$ as $n \to \infty$ can be obtained from the general theory on $M$-estimators (Van der Vaart, 2000, Chapter 5). Using this approach, we easily obtain the following proposition:

**Proposition 3.** Let $k_Y$ satisfy $|k_Y| \leq 1$, $D_n = D_n^0$ for all $n$, and assume that the following conditions hold:

- $\Theta$ is compact.
- The mapping $\theta \mapsto \mathbb{E}_{Y \mid X \sim P_{g(\theta, x)}} \left\{ k_Y(Y, Y') - 2k_Y(Y, y) \right\}$ is continuous on $\Theta$ for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$.
- The mapping $\theta \mapsto \mathbb{E}\left\{ \mathbb{D}_{k_Y}(P_{g(\theta, X_1)}), P_{Y \mid X_1}^0 \right\}$ has a unique global minimum at $\hat{\theta}_0 \in \Theta$.

Then, $\tilde{\theta}_n \to \hat{\theta}_0$ in $\mathbb{P}$-probability.

If the model is well-specified, that is if $(P^0_{Y \mid x})_{x \in \mathcal{X}} \in \{(P_{g(\theta, x)}), \theta \in \Theta\}$, then a sufficient condition for $\hat{\theta}_0$ to be well-defined is that $k_Y$ is a characteristic kernel and that the model $(P_{g(\theta, x)}), \theta \in \Theta$ is identifiable, in the sense that $\mathbb{P}(\theta_1 \neq \theta_2 \Rightarrow P_{g(\theta_1, X)} \neq P_{g(\theta_2, X)}) = 1$. It is also important to stress that, since for $\tilde{\theta}_n$ we focus on Huber’s type contaminations of the sample, in Proposition 3 there is no loss of generality to assume that $D_n = D_n^0$ for all $n$. Indeed, in the random design setting, under an $(\epsilon, Q)$-Huber contamination of the sample we have that $(X_i, Y_i) \overset{iid}{\sim} \tilde{P}^0 := \epsilon Q + (1-\epsilon)P^0$ and thus, since Proposition 3 requires no assumption on $P^0$, its result remains valid if $P^0$ is replaced by $\tilde{P}^0$. It is also worth mentioning that, unless the model is well-specified, the parameter value $\hat{\theta}_0$ defined in Proposition 3 will be typically different from the parameter value $\hat{\theta}_0$ the estimator $\hat{\theta}_n$ converges to. Finally, we note that using the general theory on $M$-estimators one can obtain sufficient conditions on $k_Y$ and on the statistical model which ensure that $\hat{\theta}_n$ is $\sqrt{n}$-consistent and asymptotically Gaussian.

The following theorem provides an asymptotic guarantee regarding the robustness of $\hat{\theta}_n$ to Huber type contaminations of the data. Notably, a direct implication of this theorem is that the influence function of $\hat{\theta}_n$ is bounded.

**Theorem 4.** Let $k_Y$ satisfy $|k_Y| \leq 1$, $Q \in \mathcal{P}(\mathcal{Z})$ and assume that following two conditions hold:

- The mapping $\theta \mapsto \mathbb{E}\left\{ \mathbb{D}_{k_Y}(P_{g(\theta, X)}), P_{Y \mid X}^0 \right\}$ has a unique global minimum at $\hat{\theta}_0$.
- There exist a neighbourhood $U$ of $\hat{\theta}_0$ and a constant $\mu > 0$ such that, for all $\theta \in U$,

$$
\mathbb{E}_{X \sim P^0_X} \left\{ \mathbb{D}_{k_Y}(P_{g(\theta, X)}), P_{Y \mid X}^0 \right\} \geq \mathbb{E}_{X \sim P^0_X} \left\{ \mathbb{D}_{k_Y}(P_{g(\hat{\theta}_0, X)}), P_{Y \mid X}^0 \right\} + \mu \|\theta - \hat{\theta}_0\|. 
$$

(15)
Let

\[ \alpha = \inf_{\theta \in U} E_{X \sim P_X} \left\{ \| k_\gamma (P_{g(\theta, X)}; P_{Y|X})^2 \| - E_{X \sim P_X} \{ \| k_\gamma (P_{g(\theta_0, X)}; P_{Y|X})^2 \| \} \right\} \in (0, 4) \]

and assume that \( \epsilon \in [0, \alpha/(52 + \alpha)) \). Then, for all

\[ \tilde{\theta}_{Q, \epsilon} \in \arg\min_{\theta \in \Theta} E_{X \sim P_X} \left\{ \| k_\gamma \{ P_{g(\theta, X)}, \epsilon Q_{Y|X} + (1 - \epsilon) P_{Y|X}^0 \}^2 \| \right\} \]

we have \( \| \tilde{\theta}_{Q, \epsilon} - \theta_0 \| \leq 52\epsilon/ (\mu - \epsilon \mu) \).

Following similar steps as in the proof of Proposition 2, it is easily checked that condition (15) holds when the function \( \theta \rightarrow E_{X \sim P_X} \{ \| k_\gamma (P_{g(\theta, X)}, P_{Y|X})^2 \| \} \) has \( \theta_0 \) as unique global minimizer and is twice continuously differentiable around this parameter value.

5. Numerical experiments

5.1. Set-up

All the results presented in this section are obtained for \( \mathcal{X} = \mathbb{R}^d \), \( \mathcal{Y} \subset \mathbb{R}^{d_y} \) for some \( d_y \in \mathbb{N} \), and for the kernel \( k = k_\gamma \otimes k_\gamma \) such that \( k_\gamma = K_{0.5, 0.01} \), i.e., \( k_\gamma \) is the exponential kernel on \( \mathbb{R}^d \) with bandwidth parameter \( \gamma = 0.01 \), and such that \( k_\gamma \) is the exponential kernel on \( \mathcal{Y} \) with bandwidth parameter equal to 1.

For each experiment the observations used to fit the model are obtained from an uncontaminated dataset \( d_0^N := \{ (x_i^0, y_i^0) \}_{i=1}^N \) that we contaminate as follows. We choose an \( \epsilon \in [0, 1) \) and randomly select a set \( I \subset \{1, \ldots, N\} \) such that \( |I| = \lfloor \epsilon N \rfloor \). For all \( i \in \{1, \ldots, N\} \) we then let \( (x_i, y_i) = (x_i^0, y_i^0) \) if \( i \notin I \) and \( (x_i, y_i) = (x_i^c, y_i^c) \) for some \( (x_i^c, y_i^c) \in \mathcal{Z} \) if \( i \in I \). The way we generate the \( (x_i^c, y_i^c) \)'s will vary from one example to the next and will therefore be specified in due course. Finally, for \( n \leq N \) we let \( d_n = \{(x_i, y_i)\}_{i=1}^n \) be the sample available to estimate the model parameter.

Below the value of the estimators \( \hat{\theta}_n \) and \( \bar{\theta}_n \) are obtained using AdaGrad (Duchi et al., 2011), an adaptive stochastic gradient algorithm, and the strategy exposed in Appendix A.2 for computing the former estimator is implemented. As suggested in Section 3.4, the algorithms that compute \( \hat{\theta}_n \) and \( \bar{\theta}_n \) use the maximum likelihood estimate of the model parameter as starting value.

5.2. Gaussian linear regression

We let \( d = 8 \) and, for every \( x \in \mathbb{R}^d \), we let \( P_{g(\theta, x)} = N(\beta^\top x, \sigma^2) \) with \( \theta = (\beta, \sigma) \in \Theta := \mathbb{R}^d \times (0, \infty) \). For this example the dataset \( d_0^N \) is constructed by simulating independent observations using

\[ Y_i^0 = \beta_0^\top X_i^0 + \epsilon_i, \quad (X_i^0, \epsilon_i) \overset{iid}{\sim} N_0(0, I_d) \otimes \text{Laplace}(0, \sigma_0) \]

with \( \beta_0 = (4, 4, 3, 3, 2, 2, 1, 1) \) and \( \sigma_0 = 1 \). The model \( \{(P_{g(\theta, x)})_{x \in \mathbb{R}^d}, \theta \in \Theta\} \) is therefore misspecified and, in what follows, we focus on the estimation of \( \beta_0 \). We let \( N = 5000 \)
| τ | type | n  | $\beta_{\text{ols},n}$ | $\beta_{\text{lad},n}$ | $\beta_{\text{rob},n}$ | $\hat{\beta}_{\text{mom},n}$ | $\tilde{\beta}_{n}$ | $\hat{\beta}_{n}$ |
|---|------|----|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| 0 |      | 100| 0.392           | 0.355           | 0.350           | 0.409           | 0.355          | 0.334          |
|    |      | 1000| 0.116          | 0.092           | 0.104           | 0.168           | 0.108          | 0.107          |
|    |      | 5000| 0.053           | 0.039           | 0.046           | 0.111           | 0.049          | 0.047          |
| 1 Y |      | 100| 0.464           | 0.339           | 0.385           | 0.707           | 0.350          | 0.342          |
|    |      | 1000| 0.181          | 0.094           | 0.106           | 0.921           | 0.105          | 0.097          |
|    |      | 5000| 0.103           | 0.043           | 0.049           | 0.807           | 0.054          | 0.051          |
| 2 Y |      | 100| 0.241           | 0.097           | 0.110           | 1.513           | 0.114          | 0.115          |
|    |      | 1000| 0.241          | 0.097           | 0.110           | 1.513           | 0.114          | 0.115          |
|    |      | 5000| 0.175           | 0.039           | 0.047           | 1.357           | 0.051          | 0.052          |
| 3 Y |      | 100| 0.724           | 0.331           | 0.343           | 1.519           | 0.329          | 0.320          |
|    |      | 1000| 0.309          | 0.100           | 0.108           | 1.864           | 0.113          | 0.110          |
|    |      | 5000| 0.250           | 0.043           | 0.048           | 1.759           | 0.053          | 0.055          |
| 1 X |      | 100| 0.870           | 0.356           | 0.374           | 0.476           | 0.342          | 0.338          |
|    |      | 1000| 0.836          | 0.111           | 0.105           | 0.254           | 0.104          | 0.096          |
|    |      | 5000| 0.818           | 0.065           | 0.049           | 0.174           | 0.054          | 0.052          |
| 2 X |      | 100| 1.575           | 0.400           | 0.347           | 0.655           | 0.337          | 0.331          |
|    |      | 1000| 1.467          | 0.160           | 0.110           | 0.319           | 0.112          | 0.115          |
|    |      | 5000| 1.401           | 0.119           | 0.046           | 0.245           | 0.051          | 0.052          |
| 3 X |      | 100| 1.838           | 0.442           | 0.344           | 0.743           | 0.331          | 0.325          |
|    |      | 1000| 1.805          | 0.216           | 0.108           | 0.377           | 0.113          | 0.109          |
|    |      | 5000| 1.771           | 0.183           | 0.048           | 0.293           | 0.054          | 0.056          |

Table 1.: Results for the Gaussian linear regression model. For each experimental setting we report the RMSE over 25 replications.

and, for $n \leq N$ and $\epsilon > 0$, the contaminated dataset $d_n$ is generated as explained in Section 5.1 where two types of outliers $(x^c_i, y^c_i)$ are considered. More precisely, we say that the outliers are of type X when $y^c_i = y_i$ and $x^c_i$ is such that $x^c_{ij} = x_{ij}$ for all $j > 1$ and such that $x^c_{i1}$ is a random draw from the $N(5, 1)$ distribution, and of type Y when $y^c_i$ is a random draw from the $N(10, 1)$ distribution and $x^c_i = x_i$.

In Table 1 we report, for different values of $n \leq N$ and of $\epsilon \in [0, 0.03]$, the root mean squared error (RMSE) for the estimation of $\beta_0$ obtained for six estimators, namely the ordinary least squares estimator $\beta_{\text{ols},n}$, the least absolute deviations estimator $\beta_{\text{lad},n}$, the robust estimator of $\beta$ in linear Gaussian regression models proposed by Koller and Stahel (2011), computed using the R package robustbase, the robust Median-of-Means estimator $\hat{\beta}_{\text{mom},n}$ introduced by Lecué et al. (2020), computed using the Python package scikit-learn-extra and using three blocks, and the two proposed estimators $\hat{\beta}_n$ and $\tilde{\beta}_n$.

When the sample is not contaminated, i.e. when $d_n = d^0_n$, we observe that the ordinary least squares estimator $\beta_{\text{ols},n}$ is the best estimator. However, this estimator is extremely sensitive to the presence of outliers of both types, a fact that is already well documented in the literature (see for example Rousseeuw and Leroy, 2005, Chapter 1). We also observe that the estimator $\hat{\beta}_{\text{mom},n}$ performs poorly, with an RMSE which is in all cases larger than that of $\beta_{\text{ols},n}$. The theory predicts that increasing the number of blocks used by the Median-of-Means procedure should make $\hat{\beta}_{\text{mom},n}$ more robust but then the

[3] https://scikit-learn-extra.readthedocs.io/en/stable/index.html
optimization procedure, as implemented in scikit-learn-extra, becomes less stable. For this reason, unreported numerical results have shown that increasing the number of blocks does not improve the empirical performance of $\hat{\beta}_{\text{mom},n}$. As predicted by our theory, the MMD based estimators $\hat{\beta}_n$ and $\tilde{\beta}_n$ are robust to the two considered types of outliers. In addition, we observe that their performance is almost identical to that of the robust estimator $\hat{\beta}_{\text{rob},n}$ proposed by Koller and Stahel (2011), and that their RMSE is in all cases smaller than that of $\hat{\beta}_{\text{lad},n}$ when the outliers are of type $X$. However, for outliers of type $Y$ this latter estimator tends to be the best one, with an RMSE slightly lower than that of the estimators $\hat{\beta}_n$, $\tilde{\beta}_n$ and $\hat{\beta}_{\text{rob},n}$.

### 5.3. Heckman sample selection model

For $d \in \mathbb{N}$ and $\Theta \subseteq \mathbb{R}^d \times (0, \infty) \times (-1, 1)$, the Heckman sample selection model $\{(P_{g(\theta,x)})_{x \in \mathbb{R}^d}, \theta \in \Theta\}$ is such that, for all $x \in \mathbb{R}^d$ and $\theta = (\beta, \gamma, \sigma, \rho) \in \Theta$, the distribution $P_{g(\theta,x)}$ is the distribution $P_{Y|x}$ defined in the last example of Proposition 1. For this model, in addition to the two MMD based estimators $\hat{\theta}_n$ and $\tilde{\theta}_n$, results are presented for $\hat{\theta}_{\text{mle},n}$, the maximum likelihood estimator of $\theta$, computed using the R package sampleSelection (Toomet et al., 2008), and for $\hat{\theta}_{\text{rob},n}$, the robust two-step estimator of $\theta$ proposed by Zhelonkin et al. (2016), computed using the R package ssmrob written by Zhelonkin et al. (2021). We stress that the estimator $\hat{\theta}_{\text{rob},n}$ is designed specifically for robust estimation in Heckman sample selection models.

We first let $d = 8$,

$$\Theta = \{(\beta, \gamma, \sigma, \rho) \in \mathbb{R}^d \times (0, \infty) \times (-1, 1) \text{ such that } \beta_{d-i+1} = \gamma_i = 0, \forall i \in \{1, \ldots, d/2\}\}$$

| $\epsilon$ | $n$ | $\hat{\theta}_{\text{mle},n}$ | $\hat{\theta}_{\text{rob},n}$ | $\hat{\theta}_n$ | $\tilde{\theta}_n$ | $\beta_0$ | $\beta_n$ |
|---|---|---|---|---|---|---|---|
| 0% | 100 | 1.504 | 2.132 | 2.012 | 2.012 | 1.451 | 1.696 |
|  | 1000 | 0.565 | 0.733 | 0.735 | 0.735 | 0.536 | 0.574 |
|  | 5000 | 0.210 | 0.296 | 0.290 | 0.289 | 0.202 | 0.238 |
| 1% | 100 | 1.776 | 2.020 | 2.017 | 1.802 | 1.598 | 1.731 |
|  | 1000 | 1.325 | 1.164 | 0.706 | 0.695 | 1.009 | 0.584 |
|  | 5000 | 1.293 | 1.083 | 0.283 | 0.283 | 0.878 | 0.273 |
| 2% | 100 | 1.766 | 1.551 | 0.683 | 0.681 | 1.938 | 1.669 |
|  | 1000 | 1.936 | 1.669 | 0.252 | 0.257 | 1.389 | 0.341 |
|  | 5000 | 2.218 | 4.131 | 2.188 | 2.147 | 1.312 | 0.638 |
| 3% | 100 | 2.657 | 3.048 | 1.786 | 1.755 | 2.200 | 1.989 |
|  | 1000 | 2.496 | 2.253 | 0.631 | 0.642 | 1.861 | 0.707 |
|  | 5000 | 2.404 | 2.142 | 0.243 | 0.242 | 1.762 | 0.418 |

Table 2.: Results for the Heckman sample selection model (synthetic data). The left table is for the estimation of $\theta = (\beta, \gamma, \sigma, \rho)$ while right table is for he estimation of $\beta$ only. For each experimental setting, we report the RMSE over 25 replications.
and construct the dataset \( d_0^N \) by simulating \( N = 5000 \) independent observations using

\[
Y_i^0 \mid X_i^0 \sim P_{g(\theta_0, X_i^0)}, \quad X_i^0 \overset{iid}{\sim} N_d(\theta_0, I_d)
\]

where \( \theta_0 = (\beta_0, \gamma_0, \sigma_0, \rho_0) \) with

\[
\beta_0 = (4, 3, 2, 1, 0, 0, 0, 0, 0), \quad \gamma_0 = (0, 0, 0, 0, 4, 3, 2, 1), \quad \sigma_0 = 1.5, \quad \rho_0 = 0.5.
\]

The model we consider here assumes that the outcome equation depends only on the first \( d/2 \) components of \( X_i^0 \) while the selection equation depends only on the last \( d/2 \) components of \( X_i^0 \), so that the total number of parameter to estimate is \( d + 2 = 10 \). For \( n \leq N \) and \( \epsilon > 0 \) the contaminated dataset \( d_n \) is constructed as explained in Section 5.1 with \( y_i^c = y_i \) and \( x_i^c \) such that \( x_i^{c,j} = x_{ij} \) for all \( j > 1 \) and such that \( x_i^{c,1} \) is a random draw from the \( N_1(5, 1) \) distribution.

Table 2 shows, for different values of \( n \leq N \) and of \( \epsilon \in [0, 0.03] \), the RMSE obtained with the different estimators for the estimation of \( \theta_0 \) as well as for the estimation of \( \beta_0 \), which is often the main parameter of interest in this model. We observe that the maximum likelihood estimator is the best estimator when there are no outliers, as expected from the asymptotic theory. On the other hand, this estimator is sensitive to the presence of outliers. The robust estimator \( \hat{\theta}_{\text{rob},n} \) of Zhelonkin et al. (2016) improves upon \( \hat{\theta}_{\text{mle},n} \) when the sample is contaminated. However, for all the considered values of \( \epsilon > 0 \) and \( n \), this estimator is dominated by \( \hat{\theta}_n \) and by \( \hat{\theta}_0 \). When restricting our attention to the estimation of \( \beta \), we observe in Table 2 that the two MMD based estimators have a lower RMSE than \( \hat{\beta}_{\text{rob},n} \) for all \( \epsilon > 0 \) when \( n = 5000 \) and for \( \epsilon = 0.03 \) when \( n = 1000 \).

We now consider the real dataset and model used in Zhelonkin et al. (2016, Table 4). The dataset, available from the R package \texttt{ssmrob}, contains \( N = 3328 \) observations
the dataset $d$ extracted from the 2001 Medical Expenditure Panel Survey, and an Heckman sample selection model is used to regress $y_{1i}$, the log ambulatory expenses for the $i$th individual, on the vector $x_{i}^{0}$ containing $d = 7$ covariates, including an intercept. Both the selection and the outcome equation is assumed to depend on all the components of $x_{i}^{0}$, so that $\Theta = \mathbb{R}^{d} \times (0, \infty) \times (-1, 1)$ and the number of parameter to estimate is $2d + 2 = 16$. We let $n = N$ and, for a given $\epsilon > 0$, we contaminate the dataset $d_{N}^{0}$, where $y_{0i} = \mathbb{I}_{(0, \infty)}(y_{1i}^{0})$, by applying the approach described in Section 5.1 with $(y_{1i}^{0}, y_{2i}^{0}, x_{i}^{0}) = (y_{1i}^{0}, 1 - y_{2i}^{0}, x_{i}^{0})$. Below we denote by $d_{n, \epsilon}$ the resulting contaminated version of $d_{n}^{0}$.

The estimated parameters values, obtained for $\epsilon \in \{0, 0.01, 0.03\}$ and the four considered estimators, are presented in Table 3. For $\epsilon = 0$ the results obtained with $\theta_{\text{mle}, n}$ and with $\theta_{\text{rob}, n}$ reproduce those given in Zhelonkin et al. (2016), and the two MMD based estimators provide similar estimated values of the model parameters. In order to assess the sensibility of the different estimators to a contamination of the data, in Table 4 we give the value of $\Delta_{\tau, n}(\theta_{n}) := \|\theta_{n}(d_{n, \epsilon}) - \hat{\theta}_{n}(d_{n}^{0})\|$ for all $\theta_{n} \in \{\theta_{\text{mle}, n}, \theta_{\text{rob}, n}, \hat{\theta}_{n}, \hat{\hat{\theta}}_{n}\}$. As expected, the maximum likelihood estimator is very sensitive to the presence of outliers and $\theta_{\text{rob}, n}$ improves upon $\theta_{\text{mle}, n}$. The most striking feature of Table 4 is the remarkable performance of $\hat{\theta}_{n}$. Notably, the value $\Delta_{\tau, n}(\hat{\theta}_{n})$ is about 2.675 times smaller than that of $\Delta_{\tau, n}(\theta_{\text{rob}, n})$ when $\epsilon = 0.01$, and about 8.5 times smaller when $\epsilon = 0.03$. For this latter value of $\epsilon$ the estimator $\hat{\theta}_{n}$ outperforms the estimator $\theta_{\text{rob}, n}$ since, in this case, $\Delta_{\tau, n}(\hat{\theta}_{n})$ is about 1.8 times smaller than $\Delta_{\tau, n}(\theta_{\text{rob}, n})$. On the contrary, when there is a small proportion of outliers, i.e. when $\epsilon = 0.01$, we observe from Table 4 that $\theta_{\text{rob}, n}$ dominates $\hat{\theta}_{n}$. We however recall that $\hat{\theta}_{n}$ depends on a kernel $k_{X}$ which is kept the same throughout this Section 5 and thus which is not optimized in any sense to the particular problem at hand.

### 5.4. Gamma regression model

With $d = 8$ and $\Theta = \mathbb{R}^{d} \times (0, \infty)$, we consider the Gamma regression model $\{ (P_{\theta}(x), x \in \mathbb{R}^{d}, \theta \in \Theta) \}$ which is such that, for all $x \in \mathbb{R}^{d}$ and $\theta = (\beta, \nu) \in \Theta$, the distribution $P_{\theta}(x)$ is the distribution $P_{\gamma x}$ defined in the fourth example of Proposition 4. For this example the dataset $d_{N}^{0}$ is obtained by simulating $N = 5000$ independent observations using $Y_{i}^{0} \mid X_{i}^{0} \sim P_{\theta_{0}}(X_{i}^{0})$ and $X_{i}^{0} \sim \mathcal{N}_{d}(0, I_{d})$, with $\theta_{0} = (1, \ldots, 1)$. Then, for every $n \leq N$ and $\epsilon \in [0, 0.03]$, the contaminated dataset $d_{n}$ is constructed as described in Section 5.1 with

| $\epsilon$ | $\theta_{\text{mle}, n}$ | $\theta_{\text{rob}, n}$ | $\hat{\theta}_{n}$ | $\hat{\hat{\theta}}_{n}$ |
|-----------|-------------------------|-------------------------|---------------------|--------------------|
| 1%        | 0.651                   | 0.107                   | 0.186               | 0.040              |
| 3%        | 1.090                   | 0.468                   | 0.259               | 0.055              |

Table 4.: Value of $\Delta_{\tau, n}(\theta_{n})$ for the Heckman sample selection model for the 2001 Medical Expenditure Panel Survey dataset, with $\theta_{n} \in \{\theta_{\text{mle}, n}, \theta_{\text{rob}, n}, \hat{\theta}_{n}, \hat{\hat{\theta}}_{n}\}$.
Table 5.: Results for the Gamma regression model. For each experimental setting, we report the mean square error over 25 replications.

| ε  | n   | θ_{mle,n} | θ_{rob,n} | θ_n | θ_n |
|----|-----|-----------|------------|-----|-----|
| 0% | 100 | 0.123     | 0.120      | 0.142 | 0.144 |
|    | 1000| 0.055     | 0.053      | 0.067 | 0.069 |
|    | 5000|           |            |       |       |
| 1% | 100 | 0.250     | 0.108      | 0.149 | 0.148 |
|    | 1000| 0.049     | 0.071      | 0.071 | 0.070 |
|    | 5000|           |            |       |       |
| 2% | 100 | 0.353     | 0.113      | 0.146 | 0.145 |
|    | 1000| 0.056     | 0.073      | 0.073 | 0.073 |
|    | 5000|           |            |       |       |
| 3% | 100 | 0.444     | 0.407      | 0.471 | 0.475 |
|    | 1000| 0.069     | 0.076      | 0.076 | 0.078 |

| ε  | n   | β_{mle,n} | β_{rob,n} | β_n | β_n |
|----|-----|-----------|------------|-----|-----|
| 0% | 100 | 0.087     | 0.093      | 0.132 | 0.133 |
|    | 1000| 0.041     | 0.043      | 0.061 | 0.063 |
|    | 5000|           |            |       |       |
| 1% | 100 | 0.114     | 0.118      | 0.132 | 0.133 |
|    | 1000| 0.070     | 0.071      | 0.071 | 0.070 |
|    | 5000|           |            |       |       |
| 2% | 100 | 0.120     | 0.129      | 0.127 | 0.127 |
|    | 1000| 0.094     | 0.094      | 0.094 | 0.094 |
|    | 5000| 0.064     | 0.064      | 0.064 | 0.064 |
| 3% | 100 | 0.119     | 0.119      | 0.138 | 0.138 |
|    | 1000| 0.091     | 0.091      | 0.091 | 0.091 |
|    | 5000| 0.044     | 0.044      | 0.044 | 0.044 |

\( y_i^c = y_i \) and \( x_i^c \) such that \( x_i^c_j = x_{ij} \) for all \( j > 1 \) and such that \( x_i^c_1 \) is a random draw from the \( N_1(-0.5, 1) \) distribution.

Table 5 presents the RMSE for the estimation of \( \theta_0 \) and \( \beta_0 \) obtained with \( \hat{\theta}_n \) and \( \tilde{\theta}_n \). Results are also given for \( \theta_{mle,n} \), the maximum likelihood estimator of \( \theta \), and for \( \theta_{rob,n} \), the estimator proposed by Cantoni and Ronchetti (2001, 2006) for robust inference in generalized linear model, computed using the \texttt{R} package \texttt{robustbase}. We observe from this table that, as expected, \( \theta_{mle,n} \) is not robust to the presence of outliers, while the two proposed MMD based estimators are. In all cases, the RMSE obtained with the estimator \( \theta_{rob,n} \) proposed by Cantoni and Ronchetti (2001, 2006) is however slightly smaller than the that obtained with \( \hat{\theta}_n \) and \( \tilde{\theta}_n \).

We stress that, in some sense, the better performance of \( \theta_{rob,n} \) is reassuring since this estimator is precisely designed for robust inference in generalized linear models and, in particular, has been motivated in Cantoni and Ronchetti (2006) for robust inference in Gamma regression models. By contrast, the applicability of the estimators \( \hat{\theta}_n \) and \( \tilde{\theta}_n \), and their theoretical guarantees derived in Section 4 regarding their robustness, hold for a much broader class of regression models.

6. Conclusion

Some important questions remain open, such as the dependence of the convergence rate of the estimator \( \hat{\theta}_n \) to the dimension of the parameter space \( \Theta \), and the existence of conditional mean embedding operators when \( \mathcal{X} \) is unbounded which would enable to apply some our theoretical results for this estimator to problems where the regressors can take arbitrarily large values. Finally, further work is needed establish non-asymptotic guarantees for the estimator \( \tilde{\theta}_n \).
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Supplementary material

Supplementary material available at Biometrika includes additional information about the computation of the two estimators and all the proofs.

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A. Computation of the estimators

A.1. Gradient of the loss

**Proposition 4.** Assume that each $P_\lambda$ has a density $p_\lambda$ with respect to a measure $\mu$ such that $\lambda \mapsto p_\lambda$ is differentiable, and that $\theta \mapsto g(\theta, x)$ is differentiable for any $x \in X$.

1. Assume that there is a function $\hat{b} : Y^2 \to \mathbb{R}$ such that
   \[
   \int_Y \hat{b}(y, y') \mu(dy) \mu(dy') < \infty,
   \]
   and such that, for all $(\theta, x, x', y, y')$,
   \[
   |k((x, y), (x', y')) \nabla_\theta p_g(\theta, x)(y)p_g(\theta', x')(y')| \leq \hat{b}(y, y').
   \]
   Then, for all $(\theta, x, x', y)$ we have
   \[
   \nabla_\theta \hat{\ell}(\theta, x, x', y) = 2 \mathbb{E}_{Y \sim p_g(\theta, x), Y' \sim p_g(\theta, x')}
   \left[
   k((x, y), (x', y')) - k((x, Y'), (x', y))
   \right]
   \nabla_\theta \log p_g(\theta, x)(Y).
   \]

2. Assume that there exists a function $\tilde{b} : Y^2 \to \mathbb{R}$ such that
   \[
   \int_Y \tilde{b}(y, y') \mu(dy) \mu(dy') < \infty
   \]
   and such that, for all $(\theta, x, y, y')$,
   \[
   |k(y, y') \nabla_\theta p_g(\theta, x)(y)p_g(\theta', x')(y')| \leq \tilde{b}(y, y').
   \]
   Then, for all $(\theta, x, y)$ we have
   \[
   \nabla_\theta \tilde{\ell}(\theta, x, y) = 2 \mathbb{E}_{Y, Y' \sim p_g(\theta, x)} \left[
   k_Y(Y, Y') - k_Y(Y, y)
   \right]
   \nabla_\theta \log p_g(\theta, x)(Y).
   \]

**Remark 5.** We need more assumption to ensure stability and convergence of the stochastic gradient algorithm. See for example Proposition 5.2 in Chérif-Abdellatif and Alquier (2022) (and the references therein), where the authors require the existence of the variance of

\[
\hat{L}(\theta, x, x', U, U'') := 2 \left(k((x, Y), (x', Y')) - k((x, Y), (x', y))\right) \nabla_\theta \log p_g(\theta, x)(Y)
\]
when $U \sim P_{g(\theta, x)}$ and $U' \sim P_{g(\theta, x')}$. However, under Assumption $[\mathcal{A}]$, it boils down to the corresponding assumption on $\nabla_\theta \log p_{g(\theta, x)}(U)$. For example, if there is $v > 0$ such that for any $(x, \theta)$, $\mathbb{E}_{U \sim P_{g(\theta, x)}}[\| \nabla_\theta \log p_{g(\theta, x)}(U) \|^2] \leq v$, then

$$\text{Var}(\tilde{L}(\theta, x, x', U, U', y)) \leq 16v, \quad \forall (\theta, x, x', y).$$

**Proof.** We start by the proof of point 2. By definition,

$$\tilde{\ell}(\theta, X_i, Y_i) = \mathbb{E}_{Y \sim P_{g(\theta, X_i)}}, Y' \sim P_{g(\theta, X_i)}} [k_{Y}(Y, Y') - 2k_{Y}(Y, Y_i)]$$

$$= \int \int [k_{Y}(y, y') - 2k_{Y}(y, Y_i)] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy')$$

$$= \int k_{Y}(y, y') p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy') - 2 \int k_{Y}(y, Y_i) p_{g(\theta, X_i)}(y) \mu(dy),$$

so that

$$\nabla_\theta \tilde{\ell}(\theta, X_i, Y_i) = \nabla_\theta \int \int k_{Y}(y, y') p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy')$$

$$- \nabla_\theta \int k_{Y}(y, Y_i) p_{g(\theta, X_i)}(y) \mu(dy)$$

$$= \int k_{Y}(y, y') \nabla_\theta \left[ p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \right] \mu(dy) \mu(dy')$$

$$- 2 \int k_{Y}(y, Y_i) \nabla_\theta \left[ p_{g(\theta, X_i)}(y) \right] \mu(dy)$$

(16)

where the inversion of $\int$ and $\nabla$ is justified thanks to the existence of the function $\tilde{b}$. Remark that

$$\nabla_\theta \left[ p_{g(\theta, X_i)}(y) \right] = \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)}$$

and that

$$\nabla_\theta \left[ p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \right]$$

$$= \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') + \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y') \right] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y').$$

Plugging this into (16) gives:

$$\nabla_\theta \tilde{\ell}(\theta, X_i, Y_i) = \int k_{Y}(y, y') \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy')$$

$$+ \int k_{Y}(y, y') \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y') \right] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy')$$

$$- 2 \int k_{Y}(y, Y_i) \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)} \mu(dy)$$

$$= 2 \int k_{Y}(y, y') \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)}(y) p_{g(\theta, X_i)}(y') \mu(dy) \mu(dy')$$

$$- 2 \sum_{i=1}^{n} \int k_{Y}(y, Y_i) \nabla_\theta \left[ \log p_{g(\theta, X_i)}(y) \right] p_{g(\theta, X_i)} \mu(dy)$$

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by symmetry, and thus,

\[ \nabla_\theta \tilde{\ell}(\theta, X_i, Y_i) = 2 \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{Y \sim P_\theta(x_i, Y)} \left\{ [k_\gamma(Y, Y') - k_\gamma(Y, Y_i)] \nabla_\theta \left[ \log p_\theta(x_i, Y) \right] \right\}. \]

The proof of point 1, from the expression in (10), is exactly similar. \( \square \)

A.2. A closer look at the computation of \( \hat{\theta}_n \)

Let \( k = k_\gamma \otimes k_\gamma \) with \( k_\gamma \) as in Section 3.3 and let \( L(\theta, x, x', y) \) be a random variable such that \( \mathbb{E}[L(\theta, x, x', y)] = \nabla_\theta \ell(\theta, x, x', y) \), with \( \ell(\theta, x, x', y) \) as defined in Section 3.3. Then, given \( n \) observations \( d_n := \{(x_i, y_i)\}_{i=1}^n \) in \( \mathcal{Z} \), the random variable

\[ H_n(\gamma, \theta, d_n) := 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} k_\gamma(x_i, x_j) L(\theta, x_i, x_j, y_j) \]

is such that \( \mathbb{E}[H_n(\gamma, \theta, d_n)] = \nabla_\theta h_n(\gamma, \theta, d_n) \), with \( h_n(\gamma, \theta, d_n) \) as defined in (10).

Next, for an integer \( M_1 \in \{1, \ldots, (n-1)n/2 - 1\} \) we let

\[ \mathcal{S}_{M_1} \subset \mathcal{S} := \{(i, j) : 1 \leq i < j \leq n\} \]

be such that the set \( \{k_\gamma(x_i, x_j)\}_{(i,j)\in\mathcal{S}_{M_1}} \) contains the \( M_1 \) largest elements of the set \( \{k_\gamma(x_i, x_j)\}_{(i,j)\in\mathcal{S}} \), and for an integer \( M_2 \in \mathbb{N} \) such that \( M_1 + M_2 \leq (n-1)n/2 \) we let \( \{(I_i, J_i)\}_{i=1}^{M_2} \) be a simple random sample obtained without replacement from the set \( \mathcal{S} \setminus \mathcal{S}_{M_1} \). Then, the random variable

\[ H_{n,M_1,M_2}^{(M_1,M_2)}(\gamma, \theta, d_n) := 2 \sum_{(i,j)\in\mathcal{S}_{M_1}} k_\gamma(x_i, x_j) L(\theta, x_i, x_j, y_j) + \frac{(n-1)n - 2M_1}{M_2} \sum_{m=1}^{M_2} k_\gamma(x_{I_m}, x_{J_m}) L(\theta, x_{I_m}, x_{J_m}, y_{J_m}) \]

is such that \( \mathbb{E}[H_{n,M_1,M_2}^{(M_1,M_2)}(\gamma, \theta, d_n)] = h_n(\gamma, \theta, d_n) \), and thus

\[ \mathbb{E} \left[ \sum_{i=1}^{N} L(\theta, x_i, y_i) + H_{n,M_1,M_2}^{(M_1,M_2)}(\gamma, \theta, d_n) \right] = \nabla_\theta \sum_{i,j=1}^{n} \ell(\theta, X_i, X_j, Y_j). \quad (17) \]

This approach for computing an unbiased estimate of \( \nabla_\theta \sum_{i,j=1}^{n} \ell(\theta, X_i, X_j, Y_j) \) involves the construction of the sets \( \mathcal{S} \) and \( \mathcal{S}_{M_1} \), which requires \( \mathcal{O}(n^2) \) operations. However, once these two sets are obtained, obtaining a realization of \( G_n(\theta, d_n) := \sum_{i=1}^{N} L(\theta, x_i, y_i) + H_{n,M_1,M_2}^{(M_1,M_2)}(\gamma, \theta, d_n) \) for a given \( \theta \) can be done in only \( \mathcal{O}(n + M_1 + M_2 \log (M_2)) \) operations using e.g. the simple random sampling without replacement method proposed by Gupta and Bhattacharjee (1984).

For this procedure to work well in practice the parameters \( M_1 \) and \( M_2 \) must be such that the variance of \( G_n(\theta, d_n) \) is small. When a small value for \( \gamma \) is chosen it is often
true that \( k_\gamma(x_i, x_j) \approx 0 \) for most pairs \((i, j) \in S\). When this happens, taking \( M_1 = \mathcal{O}(n) \) and \( M_2 \) such that \( M_2 \log(M_2) = \mathcal{O}(n) \) allows to efficiently compute \( \hat{\theta}_n \) using a stochastic gradient algorithm whose cost per iteration is linear in the sample size \( n \). However, the memory requirement the approach we just described is \( \mathcal{O}(n^2) \), which limits its applicability to moderate values of \( n \) (to \( n \) equals to a few thousands, say).

### B. Proof of Lemma 1

#### B.1. Preliminaries

We first recall the following result (see Da Prato and Zabczyk, 2014, Proposition 1.6):

**Lemma 5.** Let \( \mathcal{A} \) and \( \mathcal{B} \) be two Hilbert spaces, \( T : \mathcal{A} \to \mathcal{B} \) be a bounded linear operator and \( Z \) be a random variable taking values in \( \mathcal{A} \) and such that \( E[\|Z\|_A] < \infty \). Then \( E[T(Z)] = T(E[Z]) \).

We recall that, under Assumption A1-A2, for any probability distribution \( P \in \mathcal{P}(\mathcal{Z}) \) the mean embedding \( \mu(P) = E_{Z \sim P}[k(Z, \cdot)] \) of \( P \) is well defined in \( \mathcal{H} \), and that \( \mu(P) \) has the key property to be such that

\[
\langle f, \mu(P) \rangle_{\mathcal{H}} = \langle f, E_{Z \sim P}[k(Z, \cdot)] \rangle_{\mathcal{H}} = \langle E_{Z \sim P}[k(Z, \cdot)], f \rangle_{\mathcal{H}}, \quad \forall f \in \mathcal{H}
\]

where the second equality holds by Lemma 6 noting that for all \( f \in \mathcal{H} \) the mapping \( g \mapsto \langle f, g \rangle_{\mathcal{H}} \) is a bounded linear operator on \( \mathcal{H} \) while, under Assumption A2, \( E_{Z \sim P}[\|k(Z, \cdot)\|_H] \leq 1 \).

Recall also that the boundedness of \( k_\mathcal{X} \) and \( k_\mathcal{Y} \) (Assumption A2) implies that \( \mathcal{C}_p \) and \( \mathcal{C}_{pX} \) exist, are unique, and that they are bounded, linear operators (see Fukumizu et al., 2004, Section 3).

We then have the following result (also proved in the proof of Corollary 3 in Fukumizu et al., 2004 as well as in Klebanov et al., 2020, Theorem 4.1).

**Lemma 6.** Assume that Assumption A1-A2 and condition (3) hold. Then, \( \text{range}(\mathcal{C}_p^*) \subseteq \text{range}(\mathcal{C}_{pX}) \).

**Proof.** Let \( g \in \mathcal{H}_Y \) and \( f \in \mathcal{H}_X \). Then,

\[
\langle \mathcal{C}_p^*g, f \rangle_{\mathcal{H}_X} = \langle g, \mathcal{C}_p f \rangle_{\mathcal{H}_Y} = E_{(X,Y) \sim P}[g(Y)f(X)] = E_{X \sim P_X}[E[g(Y)|X]f(X)] = \langle E_{Y \sim P_Y}[g(Y)], \mathcal{C}_{pX} f \rangle_{\mathcal{H}_X} = \langle \mathcal{C}_{pX} E_{Y \sim P_Y}[g(Y)], f \rangle_{\mathcal{H}_X}
\]

where the fourth equality holds under (3) and the last one uses the fact that \( \mathcal{C}_{pX} \) is self-adjoint. Since \( g \in \mathcal{H}_Y \) and \( f \in \mathcal{H}_X \) are arbitrary, it follows that

\[
\mathcal{C}_p^*g = \mathcal{C}_{pX} E_{Y \sim P_Y}[g(Y)], \quad \forall g \in \mathcal{H}_Y
\]

and the proof of the lemma is complete. \( \square \)
B.2. Proof of the lemma

Proof. Let \( I : \mathcal{H}_\mathcal{X} \to \mathcal{H}_\mathcal{X} \) be the identity operator on \( \mathcal{H}_\mathcal{X} \) and \( \mathcal{P}_{\text{Ker}(C_{P_X})} : \mathcal{H}_\mathcal{H} \to \mathcal{H}_\mathcal{H} \) be the orthogonal projection on \( \text{Ker}(C_{P_X}) \). Recall that \( \mathcal{P}_{\text{Ker}(C_{P_X})} \) is a linear operator such that \( \| \mathcal{P}_{\text{Ker}(C_{P_X})} \|_o = 1 \). Therefore, the linear operator \( C_{P_X}^\dagger \mathcal{P}_{C_{P_X}} = I - \mathcal{P}_{\text{Ker}(C_{P_X})} \) is bounded. In addition, by Lemma 6, \( \text{range}(C_{P_X}^\dagger) \subseteq \text{range}(C_{P_X}) \) and therefore \( C_{P_X}^\dagger C_{P}^* : \mathcal{H}_\mathcal{Y} \to \mathcal{H}_\mathcal{X} \) is a bounded linear operator (Arias and Gonzalez, 2009, Theorem 2.3). Hence, recalling that if \( A : \mathcal{H}_1 \to \mathcal{H}_2 \) is a bounded linear operator between two Hilbert spaces then \( \| A^* \|_{\mathcal{H}_2} = \| A \|_{\mathcal{H}_1} \), it follows that \( (C_{P_X}^\dagger C_{P}^*)^* : \mathcal{H}_\mathcal{X} \to \mathcal{H}_\mathcal{Y} \) is a bounded linear operator.

To proceed further let \( g \in \mathcal{H}_\mathcal{Y} \) and \( f \in \mathcal{H}_\mathcal{X} \). Then,

\[
\begin{align*}
< f, C_{P_X} E_{Y \sim P_Y} [g(Y)] >_{\mathcal{H}_\mathcal{X}} &= E_{X \sim P_X} [f(X) E[g(Y)|X]] \\
&= E_{(X,Y) \sim P_{X,Y}} [g(Y)f(X)] \\
\end{align*}
\]

while, on the other hand, recalling that \( f' = C_{P_X} C_{P_X}^\dagger f' \) for all \( f' \in \text{range}(C_{P_X}) \), and recalling that \( \text{range}(C_{P_X}^\dagger) \subseteq \text{range}(C_{P_X}) \) by Lemma 6,

\[
< f, C_{P_X} C_{P_X}^\dagger C_{P}^* g >_{\mathcal{H}_\mathcal{X}} = < f, C_{P}^* g >_{\mathcal{H}_\mathcal{X}}.
\]

Hence, by (18)-(19), it follows that

\[
< f, C_{P_X} (E_{Y \sim P_Y} [g(Y)] - C_{P_X}^\dagger C_{P}^* g) >_{\mathcal{H}_\mathcal{X}} = 0
\]

and thus

\[
E_{X \sim P_X} \left[ f(X) (E_{Y \sim P_Y} [g(Y)] - C_{P_X}^\dagger C_{P}^* g)(X) \right] = < f, C_{P_X} (E_{Y \sim P_Y} [g(Y)] - C_{P_X}^\dagger C_{P}^* g) >_{\mathcal{H}_\mathcal{X}} = 0.
\]

Consequently, since \( f \in \mathcal{H}_\mathcal{X} \) is arbitrary, it follows that, under the assumptions of the lemma,

\[
E_{Y \sim P_Y} [g(Y)] = C_{P_X}^\dagger C_{P}^* g
\]

(20)

Remark now that for \( x \in \mathcal{X} \) and \( y \in \mathcal{Y} \) we have

\[
C_{P_X}^\dagger C_{P}^* k_X(y, \cdot)(x) = < C_{P_X}^\dagger C_{P}^* k_Y(y, \cdot), k_X(x, \cdot) >_{\mathcal{H}_\mathcal{X}} = k_Y(y, \cdot), (C_{P_X}^\dagger C_{P})^* k_X(X, \cdot) >_{\mathcal{H}_\mathcal{Y}} = (C_{P_X}^\dagger C_{P})^* k_X(x, \cdot)(y)
\]

(21)

where the first equality uses the reproducing property of \( k_X \) and the third equality the reproducing property of \( k_Y \).
Let \( y \in Y \) and \( x \in X \). Then, using (20) with \( g = k_Y(y, \cdot) \) and (21), we have

\[
\mu(P_{Y|X}(y)) = \mathbb{E}_{Y \sim P_{Y|X}}[k_Y(y, Y)] \\
= C_X^t C_P^t k_Y(y, \cdot)(x) \\
= (C_X^t C_P^t)^* k_X(x, \cdot)(y)
\]

and the proof is complete. \( \square \)

C. Proof of Theorem 1

C.1. A preliminary result for proving Theorem 1

Lemma 7. Assume that \(|k_X| \leq 1\) and let \( \mu(dy) \) be a \( \sigma \)-finite measure on \((Y, \mathcal{S}_Y)\) and \( f : \mathcal{X} \times Y \to \mathbb{R} \) be such that

1. \( f(\cdot, y) \in \mathcal{H}_X \) for all \( y \in Y \),
2. The function \( \mathcal{Y} \ni y \mapsto f(\cdot, y) \) is Borel measurable,
3. The set \( \{ f(\cdot, y) : y \in \mathcal{Y} \} \) is separable,
4. \( \int_Y \| f(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) < \infty \).

Then, \( \int_Y f(\cdot, y) \mu(dy) \in \mathcal{H}_X \).

Proof. Since the set \( \{ f(\cdot, y) : y \in \mathcal{Y} \} \) is separable and the mapping \( y \mapsto f(\cdot, y) \) is Borel measurable the function \( y \mapsto f(\cdot, y) \) is strongly measurable. Therefore, there exist (Cohn, 2013, Proposition E.2) a sequence \( \{ E_{i,n} \}_{n=1}^\infty \) and a sequence \( \{ f_{i,n} \}_{n=1}^\infty \) such that

1. \( E_{i,n} \in \mathcal{S}_Y \) and \( f_{i,n} \in \mathcal{H}_X \) for all \( n \geq i \geq 1 \),
2. \( \lim_{n \to 0} \| \sum_{i=1}^n 1_{E_{i,n}}(y)f_{i,n} - f(y, \cdot) \|_{\mathcal{H}_X} = 0 \) for all \( y \in \mathcal{Y} \),
3. \( \| \sum_{i=1}^n 1_{E_{i,n}}(y)f_{i,n} \|_{\mathcal{H}_X} \leq \| f(y, \cdot) \|_{\mathcal{H}_X} \) for all \( n \geq 1 \) and all \( y \in \mathcal{Y} \).

For every \( n \geq 1 \) let \( f_n : \mathcal{X} \times Y \to \mathbb{R} \) be defined by

\[
f_n(x, y) = \sum_{i=1}^n 1_{E_{i,n}}(y)f_{i,n}(x), \quad (x, y) \in \mathcal{X} \times Y.
\]

Under the assumptions of the lemma we have \( \int_Y \| f(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) < \infty \), and thus,

\[
\int_Y \| f_n(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) \leq \int_Y \| f(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) < \infty, \quad \forall n \geq 1,
\]

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showing that, for all $n \geq 1$, the simple function $y \mapsto f_n(\cdot, y)$ is Bochner integrable. Consequently, for all $n \geq 1$ the function

$$\hat{f}_n := \int_Y f_n(\cdot, y) \mu(dy) = \sum_{i=1}^{n} \left( \int_{E_{i,n}} \mu(dy) \right) f_{i,n}$$

is well-defined. Notice that $\hat{f}_n \in \mathcal{H}_X$ for all $n \geq 1$.

To proceed further remark that $|f_n(x, y)| \leq \| f_n(\cdot, y) \|_{\mathcal{H}_X} \leq \| f(\cdot, y) \|_{\mathcal{H}_X}$, $\forall (x, y) \in X \times Y$ where the first inequality holds since $|k_X| \leq 1$ by assumption while the second inequality holds by the third aforementioned properties of $(\{E_{i,n}\}_{i=1}^{n})_{n \geq 1}$ and $(\{f_{i,n}\}_{i=1}^{n})_{n \geq 1}$.

By assumption, $\int_Y \| f(\cdot, y) \|_{\mathcal{H}_X} dy < \infty$ and thus, by the dominated converge theorem, and using the fact that the convergence in $\| \cdot \|_{\mathcal{H}_X}$ norm implies the point-wise convergence,

$$\lim_{n \to \infty} \hat{f}_n(s) = \int_Y f(s, y) dy, \; \forall s \in X. \quad (22)$$

Therefore, recalling that $\hat{f}_n \in \mathcal{H}_X$ for all $n \geq 1$, to complete the proof it remains to show that the sequence $(\hat{f}_n)_{n \geq 1}$ is Cauchy w.r.t. the $\| \cdot \|_{\mathcal{H}_X}$ norm.

To this aim remark that, since

$$\| f_n(\cdot, y) - f(\cdot, y) \|_{\mathcal{H}_X} \leq 2\| f(\cdot, y) \|_{\mathcal{H}_X}, \; \forall n \geq 1$$

while, by assumption, $\int_Y \| f(\cdot, y) \|_{\mathcal{H}_X} dy < \infty$, the dominated convergence theorem implies that

$$\lim_{n \to \infty} \int_Y \| f_n(\cdot, y) - f(\cdot, y) \|_{\mathcal{H}_X} dy = 0. \quad (23)$$

On the other hand, for every $n > m \geq 1$ we have

$$\| \hat{f}_n - \hat{f}_m \|_{\mathcal{H}_X} = \left\| \int_Y \{ f_n(\cdot, y) - f_m(\cdot, y) \} \mu(dy) \right\|_{\mathcal{H}_X} \leq \int_Y \| f_n(\cdot, y) - f_m(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) \leq \int_Y \| f_n(\cdot, y) - f(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) + \int_Y \| f_m(\cdot, y) - f(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) \quad (24)$$

where the first inequality holds by Cohn [2013, Proposition E.5], since a shown above the function $y \mapsto f_n(\cdot, y)$ is Bochner integrable. Together, (23) and (24) show that the sequence $(\hat{f}_n)_{n \geq 1}$ is indeed Cauchy w.r.t. the $\| \cdot \|_{\mathcal{H}_X}$ norm, and the proof of the lemma is complete. \qed
C.2. Proof of Theorem 1

Proof. Let \( g \in \mathcal{H}_Y \) so that \( g = \sum_{i=1}^\infty a_i k_Y(y_i, \cdot) \) for a sequence \((y_i)_{i \geq 1}\) in \( \mathcal{Y} \) and a sequence \((a_i)_{i \geq 1}\) in \( \mathbb{R} \). For all \( n \geq 1 \) let \( g_n = \sum_{i=1}^n a_i k_Y(y_i, \cdot) \) and \( f_n : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) be defined by \( f_n(x, y) = g_n(y)p(y|x), (x, y) \in \mathcal{X} \times \mathcal{Y} \). We first show that, for all \( n \geq 1 \), the function \( f_n \) verifies the assumptions of Lemma 7.

By Conditions 4 and 5 of the theorem, it readily follows that \( f_n \) verifies Conditions 4 and 5 of Lemma 7 for all \( n \geq 1 \). To show that this is also the case for Condition 2 of Lemma 7 let \( \mathcal{B}(\mathcal{H}_X) \) be the Borel \( \sigma \)-algebra on \( \mathcal{H}_X \). Let \( n \geq 1 \) and assume first that \( \mathcal{H}_X \) contains the non-zero constant functions so that the function \( y \mapsto g_n(y) \) is \( \mathcal{B}(\mathcal{H}_X) \)-measurable. Then, since by assumption the function \( y \mapsto p(y|\cdot) \) is \( \mathcal{B}(\mathcal{H}_X) \)-measurable and since the product of two Borel measurable functions is a Borel measurable function, it follows that the function \( \mathcal{Y} \ni y \mapsto f_n(\cdot, y) \) is \( \mathcal{B}(\mathcal{H}_X) \)-measurable, as required. Assume now that \( \mathcal{H}_X \) does not contain the non-zero constant functions. Let \( \tilde{\mathcal{H}}_X \) be the RKHS on \( \mathcal{X} \) having \( k_X + 1 \) as reproducing kernel so that, as shown above, the function \( \mathcal{Y} \ni y \mapsto f_n(\cdot, y) \) is \( \mathcal{B}(\tilde{\mathcal{H}}_X) \)-measurable. Consequently,

\[
\{ y \in \mathcal{Y} : f_n(\cdot|y) \in A \} \in \mathcal{G}_Y, \quad \forall A \in \mathcal{B}(\mathcal{H}_X). \tag{25}
\]

Recalling that \( \tilde{\mathcal{H}}_X = \{ f + c, f \in \mathcal{H}_X, c \in \mathbb{R} \} \) and that \( \| f \|_{\tilde{\mathcal{H}}_X} = \| f \|_{\mathcal{H}_X} \) for all \( f \in \mathcal{H}_X \) (Paulsen and Raghupathi [2016], Theorem 5.1), it follows that \( \mathcal{B}(\mathcal{H}_X) \subset \mathcal{B}(\tilde{\mathcal{H}}_X) \) which, together with (25), implies that

\[
\{ y \in \mathcal{Y} : f_n(\cdot|y) \in A \} \in \mathcal{G}_Y, \quad \forall A \in \mathcal{B}(\tilde{\mathcal{H}}_X).
\]

This shows that the function \( \mathcal{Y} \ni y \mapsto f_n(\cdot, y) \) is \( \mathcal{B}(\tilde{\mathcal{H}}_X) \)-measurable, and thus, for all \( n \geq 1, f_n \) satisfies Condition 2 of Lemma 7.

Lastly, using the fact that \( |k_Y| \leq 1 \) and Condition 4 of the theorem, for all \( n \geq 1 \) we have

\[
\int\mathcal{Y} \| f_n(\cdot, y) \|_{\mathcal{H}_X} \mu(dy) \leq \left( \sup_{y \in \mathcal{Y}} |g_n(y)| \right) \int\mathcal{Y} \| p(y|\cdot) \|_{\mathcal{H}_X} \mu(dy)
\]

\[
\leq \| g_n \|_{\mathcal{H}_Y} \int\mathcal{Y} \| p(y|\cdot) \|_{\mathcal{H}_X} \mu(dy)
\]

\[
< \infty
\]

and thus, for all \( n \geq 1, f_n \) verifies Condition 4 of Lemma 7 which concludes to show that, for all \( n \geq 1, f_n \) verifies all the assumptions of Lemma 7.

Therefore, by Lemma 7, the function \( \hat{f}_n := \int\mathcal{Y} f_n(\cdot, y) \mu(dy) \) exists and belongs to \( \mathcal{H}_X \), for all \( n \geq 1 \). In addition, for all \( m > n \geq 1 \) we have (see Cohn [2013], Proposition E.5,
for the first inequality)
\[
\|\tilde{f}_n - \tilde{f}_m\|_{\mathcal{H}_X} = \|\int_Y (g_n - g_m)(y)p(y|\cdot)\mu(dy)\|_{\mathcal{H}_X} \\
\leq \int_Y |g_n(y) - g_m(y)|\|p(y|\cdot)\|_{\mathcal{H}_X} \mu(dy) \\
\leq \sup_{y\in Y}|g_n(y) - g_m(y)|\int_Y \|p(y|\cdot)\|_{\mathcal{H}_X} \mu(dy)
\]
where, since \(|k_Y| \leq 1\) by assumption,
\[
\limsup_{n\to\infty} \sup_{m>n} \sup_{y\in Y}|g_n(y) - g_m(y)| \leq \limsup_{n\to\infty} \sup_{m>n} \|g_n - g_m\|_{\mathcal{H}_Y} = 0.
\tag{26}
\]
Consequently, the sequence \((\tilde{f}_n)_{n\geq 1}\) is Cauchy w.r.t. the \(\| \cdot \|_{\mathcal{H}_X}\) norm and therefore converges point-wise to a function \(\tilde{f} \in \mathcal{H}_X\). Thus, to complete the proof it remains to show that
\[
\lim_{n\to\infty} \tilde{f}_n(x) = E_{Y \sim P_{Y|X=x}}[g(Y)], \quad \forall x \in \mathcal{X}.
\]
Since for every \(n \geq 1\) and \(x \in \mathcal{X}\) we have
\[
|\tilde{f}_n(x) - E_{Y \sim P_{Y|X=x}}[g(Y)]| \leq \int_Y |g_n(y) - g(y)|p(y|x)\mu(dy) \leq \sup_{y\in Y}|g_n(y) - g(y)|,
\]
it follows, by (26), that \(\lim_{n\to\infty} \sup_{x\in \mathcal{X}} |\tilde{f}_n(x) - E_{Y \sim P_{Y|X=x}}[g(Y)]| = 0\), and the proof of the theorem is complete.

**D. Proof of Corollary 1**

Corollary 1 is a direct consequence of Lemma 1, Theorem 1 and of the following lemma:

**Lemma 8.** Assume that Assumptions A1-A2 hold and that there exists a \(\sigma\)-finite measure \(\mu(dy)\) on \((\mathcal{Y}, \mathcal{S}_Y)\) such that \(P_{Y|X} = p(y|x)\mu(dy)\) for all \(x \in \mathcal{X}\), where \(p(\cdot|\cdot)\) satisfies Assumptions 1-4 of Theorem 1. Moreover, assume that there exists a bounded conditional mean embedding operator \(C_{Y|X}\) for \((P_{Y|X})_{x\in \mathcal{X}}\). Then, \(\|C_{Y|X}\|_0 \leq \int_Y \|p(y|\cdot)\|_{\mathcal{H}_X} \mu(dy)\).

**Proof.** Let \(g \in \mathcal{H}_Y\) and remark that
\[
(C_{Y|X}^*g)(x) = \langle C_{Y|X}^*g, k_X(x, \cdot) \rangle_{\mathcal{H}_X} = \langle g, C_{Y|X}k_X(x, \cdot) \rangle_{\mathcal{H}_Y} = E_{Y \sim P_{Y|X=x}}[g(Y)], \quad \forall x \in \mathcal{X}
\]
where the first equality uses the reproducing property of \(k_X\) and the third \(34\).
Consequently,
\[
\|C\|_{\mathcal{H}_X} = \left\| \int_Y g(y)p(y|\cdot)dy \right\|_{\mathcal{H}_X}
\leq \int_Y \|g(y)p(y|\cdot)\|_{\mathcal{H}_X} dy \\
\leq \sup_{y \in Y} |g(y)| \int_Y \|p(y|\cdot)\|_{\mathcal{H}_X} dy \\
\leq \|g\|_{\mathcal{H}_X} \int_Y \|p(y|\cdot)\|_{\mathcal{H}_X} dy
\]
where, under the assumptions of the lemma, the first inequality holds by Cohn (2013, Proposition E.5) and where the last inequality uses the fact that \(|k_Y| \leq 1\).

Therefore,
\[
\|C\|_{\mathcal{H}_X} = \|C^*\|_{\mathcal{H}_X} \leq \int_Y \|p(y|\cdot)\|_{\mathcal{H}_X} dy
\]
and the proof of the lemma is complete.

\[\square\]

E. A useful corollary of Theorem 1

In order to state the next result we let \(\Lambda_d(dx)\) denote the Lebesgue measure on \(\mathbb{R}^d\), \(A_s = \{ \tilde{a} \in \mathbb{N}_0^d : \sum_{i=1}^d \tilde{a}_i \leq s \} \) for all \(s \in \mathbb{N}_0\) and \(|a| = \sum_{i=1}^d a_i\) for all \(a \in \mathbb{R}^d\).

**Corollary 2.** Assume that \(X \subseteq \mathbb{R}^d\) is bounded with Lipschitz boundary and, for some constants \(m \in \mathbb{N}\) and \(\gamma > 0\), let \(k_X\) be the restriction of the Matérn kernel \(K_{m,\gamma}\) on \(X \times X\).

Let \(s = (d + m)/2\) if \((d + m)\) is even and \(s = (d + m + 1)/2\) if \((d + m)\) is odd, and assume that there exists a \(\sigma\)-finite measure \(\mu(dy)\) on \((\mathcal{Y}, \mathcal{S}_Y)\) such that \(P_\mathcal{Y|X}(x) = p(y|x)\mu(dy)\) for all \(x \in X\), where \(p(\cdot|\cdot)\) satisfies the following conditions:

- for all \(y \in \mathcal{Y}\), the function \(p(y|\cdot)\) is \(s\) times continuously differentiable on \(X\), with

\[
\max_{a \in A_s} \sup_{(x,y) \in X \times Y} \left| \frac{\partial^{\sum_{i=1}^d a_i}}{\partial x_1^{a_1} \ldots \partial x_d^{a_d}} p(y|x) \right| < \infty
\]

and with

\[
\max_{a \in A_s} \int_Y \left[ \int_X \left\{ \frac{\partial^{\sum_{i=1}^d a_i}}{\partial x_1^{a_1} \ldots \partial x_d^{a_d}} p(y|x) \right\}^2 \Lambda_d(dx) \right]^{\frac{1}{2}} \mu(dy) < \infty, \quad \forall a \in A_s,
\]

- the function \(y \mapsto \frac{\partial^{\sum_{i=1}^d a_i}}{\partial x_1^{a_1} \ldots \partial x_d^{a_d}} p(y|x)\) is continuous on \(\mathcal{Y}\), for all \(x \in X\) and \(a \in A_s\).

Assume also that the set \(\mathcal{Y}\) is separable and that Assumptions A1-A2 hold. Then, conditions 1-4 of Theorem 1 hold and thus (3) is satisfied.
Proof. Remark first that to prove the result it is enough to consider the case where \((m + d)\) is even. Indeed, if \((m + d)\) is odd then in what follows we can replace
- the set \(\mathcal{X}\) by \(\tilde{\mathcal{X}} = \mathcal{X} \times \mathbb{R}^1\),
- for all \(y \in \mathcal{Y}\), the function \(p(y|\cdot) : \mathcal{X} \to \mathbb{R}\) by the function \(\tilde{p}(y|\cdot) : \tilde{\mathcal{X}} \to \mathbb{R}\) defined by \(\tilde{p}(y|(x, v')) = p(y|x)\) for all \((x, u) \in \tilde{\mathcal{X})\),
- \(d\) by \(\tilde{d} = d + 1\).

Recall that, since \((m + d)\) is even, the RKHS \(\mathcal{H}_\mathcal{X}\) is norm-equivalent to the Sobolev space \(W^s_2(\mathcal{X})\) (see e.g. Kanagawa et al., 2018, Example 2.6). In addition, recall that the norm \(\| \cdot \|_{W^s_2(\mathcal{X})}\) is defined by

\[
\|f\|_{W^s_2(\mathcal{X})} = \sum_{a \in A_s} \left( \int_{\mathcal{X}} \left| \frac{\partial^{\sum_{i=1}^{\tilde{d}} a_i} f(x)}{\partial u_1^{a_1} \ldots \partial u_{\tilde{d}}^{a_{\tilde{d}}}} \right|^2 \Lambda_d(dx) \right)^{\frac{1}{2}}, \quad f \in W^s_2(\mathcal{X})
\]

and let

\[
D_a p(y|x) = \frac{\partial^{\sum_{i=1}^{\tilde{d}} a_i} p(y|x)}{\partial u_1^{a_1} \ldots \partial u_{\tilde{d}}^{a_{\tilde{d}}}}, \quad \forall (a, x, y) \in A_s \times \mathcal{X} \times \mathcal{Y}.
\]

To prove the corollary remark first that, under its assumptions, for all \(y \in \mathcal{Y}\) we have \(\|p(\cdot|y)\|_{W^s_2(\mathcal{X})} < \infty\). Thus, for all \(y \in \mathcal{Y}\), the function \(p(y|\cdot)\) belongs to the Sobolev space \(W^s_2(\mathcal{X})\), and thus to the RKHS \(\mathcal{H}_\mathcal{X}\). This shows that \(p(\cdot|\cdot)\) verifies Condition 1 of Theorem 1.

In addition, under the assumptions of the corollary we have

\[
\int_{\mathcal{Y}} \|p(y|\cdot)\|_{W^s_2(\mathcal{X})} \mu(dy) = \sum_{a \in A_s} \int_{\mathcal{Y}} \left\{ \int_{\mathcal{X}} D_a p(y|x)^2 \Lambda_d(dx) \right\}^{\frac{1}{2}} \mu(dy) < \infty \quad (27)
\]

and thus, since the norm \(\| \cdot \|_{\mathcal{H}_\mathcal{X}}\) is equivalent to the norm \(\| \cdot \|_{W^s_2(\mathcal{X})}\), it follows that

\[
\int_{\mathcal{Y}} \|p(y|\cdot)\|_{\mathcal{H}_\mathcal{X}} \mu(dy) < \infty
\]

showing that \(p(\cdot|\cdot)\) verifies Condition 4 of Theorem 1.

To proceed further recall that the image of a separable space by a continuous function is separable. Hence, since \(\mathcal{Y}\) is assumed to be separable, to show that Condition 3 of Theorem 1 holds it suffices to show that, for every \(y' \in \mathcal{Y}\), the function

\[
\mathcal{Y} \ni y \mapsto k_{\mathcal{Y}}(y', y)p(y|\cdot) \in \mathcal{H}_\mathcal{X} \quad (28)
\]

is continuous. To this aim, let \(y' \in \mathcal{Y}\) and \((y'_i)_{i \geq 1}\) be a sequence in \(\mathcal{Y}\) such that \(\lim_{i \to \infty} y'_i = y'\). Then, since \(k_{\mathcal{Y}}\) is continuous by assumption, to show that the function defined in (28) is continuous it is enough to show that

\[
\limsup_{i \to \infty} \|p(y'_i|\cdot) - p(y'|\cdot)\|_{\mathcal{H}_\mathcal{X}} = 0. \quad (29)
\]

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The norm $\| \cdot \|_{P_X}$ being norm-equivalent to the norm $\| \cdot \|_{W^2(P_X)}$, there exists a constant $C < \infty$ such that $\|f\|_{P_X} \leq C\|f\|_{W^2(P_X)}$ for all $f \in P_X$ and thus, for all $i \geq 1$, we have

$$
\|p(y'_i|\cdot) - p(y'_i|\cdot)\|^2_{P_X} \leq C^2\|p(y'_i|\cdot) - p(y'_i|\cdot)\|^2_{W^2(P_X)}
$$

$$
\leq C^2 \sum_{a \in A_d} \int_{\mathcal{X}} |D_a p(y'_i|x) - D_a p(y'_i|x)|^2 \Lambda_d(dx).
$$

(30)

By assumption, for all $x \in \mathcal{X}$ and all $a \in A_d$, the function $y \mapsto D_a p(y|x)$ is continuous on $\mathcal{Y}$ while, for all $(a, x) \in A_d \times \mathcal{X}$ we have

$$
\sup_{i \geq 1} |D_a p(y'_i|x) - D_a p(y'_i|x)|^2 \leq 2 \sup_{(x,y) \in \mathcal{X} \times \mathcal{Y}} |D^a p(y|x)| < \infty.
$$

Consequently, since $\mathcal{X}$ is bounded, (29) follows from (30) and the dominated convergence theorem, and thus $p(\cdot|\cdot)$ satisfies Condition 3 of Theorem 1.

Finally, since as shown above the mapping $\mathcal{Y} \ni y \mapsto p(y|\cdot)$ is continuous, it follows that this mapping is Borel measurable and thus $p(\cdot|\cdot)$ satisfies Condition 2 of Theorem 1. Hence, all the conditions of Theorem 1 and the proof is complete.

\[\square\]

F. Proof of Proposition 1

F.1. Preliminary result

Lemma 9. Assume that $\mathcal{X} \subseteq \mathbb{R}^d$ for some integer $d$ and that $\mathcal{X}$ is path-wise connected and such that $\Lambda_d(\mathcal{X}) > 0$. Assume also that $k_{\mathcal{X}}$ is continuous on $\mathcal{X}^2$. Then, there exists a distribution $P_X \in \mathcal{P}(\mathcal{X})$ such that

$$
\{ f \in H_{\mathcal{X}} : \mathbb{E}_{X \sim P_X} [f(X)h(X)] = 0, \forall h \in \mathcal{X} \} = \{0\}.
$$

(31)

Proof. Remark first that since $k_{\mathcal{X}}$ is continuous on $\mathcal{X}^2$ any function $f \in H_{\mathcal{X}}$ is continuous on $\mathcal{X}$ (Paulsen and Raghupathi, 2016, Theorem 2.17). Let $P_X$ denote the $N_d(0, I_d)$ distribution, truncated on $\mathcal{X}$ if $\mathcal{X} \neq \mathbb{R}^d$. Assume that there exists a non-zero function $f \in H_{\mathcal{X}}$ such that

$$
\mathbb{E}_{X \sim P_X} [f(X)h(X)] = 0, \quad \forall h \in H_{\mathcal{X}}.
$$

Then, $\mathbb{E}_{X \sim P_X} [f(X)^2] = 0$ and, since $P_X$ admits a strictly positive density $p_X$ on $\mathcal{X}$ w.r.t. $\Lambda_d$, we have $f(x) = 0$ for $\Lambda_d$-almost every $x \in \mathcal{X}$. However, as $f$ is assumed to be continuous, and $\mathcal{X}$ is path-wise connected, the function $f$ is zero everywhere.

\[\square\]

F.2. Proof of the proposition

Proof:

The fact that $k$ is characteristic follows from Szabó and Sriperumbudur (2018) and the properties of the Matérn kernel.

Next, remark that, by Lemma 9 under the assumption of the proposition there exists a distribution $P_X \in \mathcal{P}(\mathcal{X})$ such that the only function $f \in H_{\mathcal{X}}$ for which we have
$E_{X \sim P_X}[f(X)^2] = 0$ is the zero function. In addition, since $X$ is bounded with Lipschitz boundary we can use Corollary 2 to check that there exists a bounded linear conditional mean operator for $(P_{Y|x})_{x \in X}$.

To this aim, for all $x \in X$ we let $p(y|x)$ be the density of $P_{Y|x}(dy)$ w.r.t. $\mu(dy)$. The $\sigma$-finite measure $\mu(dy)$ on $Y$ will be specified below for each example but, for all the considered examples, for all $y \in \Theta \times Y$ the mapping $x \mapsto p(y|x)$ is infinitely many times differentiable. Consequently, letting $s$ and $A_s$ be as defined in Corollary 2, we can define

$$D^a p(y|x) = \partial_{x_1^{a_1}} \cdots \partial_{x_d^{a_d}} p(y|x), \quad \forall (a, x, y) \in \Theta \times A_s \times X \times Y.$$ 

Then, by Corollary 2 a bounded linear conditional mean operator for $(P_{Y|x})_{x \in X}$ exists if

1. the mapping $y \mapsto D^a p(y|x)$ is continuous for all $(a, x) \in A_s \times X$,

2. the following two conditions hold:

$$\max_{a \in A_s} \sup_{(x, y) \in \Theta \times Y} |D^a p(y|x)| < \infty$$

$$\max_{a \in A_s} \int_Y \left[ \int_X \{D^a p(y|x)\}^2 \mu(dx) \right]^{\frac{1}{2}} \mu(dy) < \infty.$$ 

For all the examples considered in the proposition it is trivial to see that the mapping $y \mapsto D^a p(y|x)$ is continuous for all $(a, x) \in A_s \times X$. Under the assumptions made on $X$, Conditions (32) and (33) are easily checked from the definition of $p(y|x)$ given below for each examples

**Example 1:** For this example $Y = \mathbb{R}$ and we let $\mu(dy)$ be the Lebesgue measure on $\mathbb{R}$ so that

$$p(y|x) = \sum_{m=1}^{M} w_m \frac{1}{\sqrt{2\pi \sigma_m^2}} \exp \left\{ - \frac{(y - \beta_m^\top x)^2}{2\sigma_m^2} \right\}, \quad \forall (x, y) \in \Theta \times Y.$$ 

**Example 2:** For this example, $Y = \mathbb{N}_0$ and we let $\mu(dy)$ be the counting measure on $\mathbb{N}_0$ so that

$$p(y|x) = \frac{\exp \left\{ y \beta^\top x - \exp(\beta^\top x) \right\}}{y!}, \quad \forall (x, y) \in \Theta \times Y.$$ 

**Example 3:** For this example, $Y = \{0, 1\}$ and we let $\mu(dy)$ be the counting measure on $\{0, 1\}$ so that

$$p(y|x) = \left( \frac{1}{1 + \exp(-\beta^\top x)} \right)^y \left( \frac{1}{1 + \exp(\beta^\top x)} \right)^{1-y}, \quad \forall (x, y) \in \Theta \times Y.$$
Example 4: For this example, \( Y = (0, \infty) \) and we let \( \mu(dy) \) be the Lebesgue measure on \( \mathbb{R} \) so that
\[
p(y|x) = \frac{1}{\Gamma(\nu)} y^{\nu-1} \exp(-\nu \beta^\top x) \exp\{ -\nu y \exp(-\beta^\top x) \}, \quad \forall (x, y) \in \mathcal{X} \times \mathcal{Y}.
\]

Example 5: For this example, \( Y = \mathbb{R} \times \{0, 1\} \) and we let
\[
\mu(dy) = (\Lambda_1(dy_1) + \delta_{\{0\}}(dy_1)) \otimes \delta_{\{0\}}(dy_2)
\]
so that
\[
P_\lambda(dy) = \check{p}_\lambda(y) \mu(dy)
\]
where, denoting by \( \phi(\cdot; \mu, \sigma^2) \) the probability density function of the \( \mathcal{N}_1(\mu, \sigma^2) \) distribution w.r.t. \( \Lambda_1 \), for all \( (x, y) \in \mathcal{X} \times \mathcal{Y} \) we have
\[
p(y|x) = \phi(y_1; \beta^\top x, \sigma^2) \Phi\left( \frac{\{\gamma^\top x + (\rho/\sigma)\beta^\top x\}/\sqrt{1-\rho^2}\}1_{\mathbb{R}\setminus\{0\}}(y_1)(1 - 1_{\{0\}}(y_2)) \right.
\]
\[
+ \Phi(-\gamma^\top x)1_{\{0\}}(y_1)1_{\{0\}}(y_2).
\]

G. Proof of Lemma 2

Proof. Let \( \mathcal{C}_{Y|X} : \mathcal{H}_X \to \mathcal{H}_Y \) be a bounded linear operator such that
\[
\mu(P_{Y|x}) = \mathcal{C}_{Y|X} k_X(x, \cdot), \quad \forall x \in \mathcal{X}.
\]
and let \( \tilde{\mathcal{C}}_{P_{Y|x}} : \mathcal{H}_X \otimes \mathcal{H}_X \to \mathcal{H} \) be the (unique) linear operator on \( \mathcal{H}_X \otimes \mathcal{H}_X \) such that
\[
\tilde{\mathcal{C}}_{P_{Y|x}}(f_1 \otimes f_2) = f_1 \otimes \mathcal{C}_{Y|X} f_2, \quad f_1 \in \mathcal{H}_X, f_2 \in \mathcal{H}_X.
\]
For all \( f_1 \in \mathcal{H}_X \) and \( f_2 \in \mathcal{H}_X \) we have
\[
\|\tilde{\mathcal{C}}_{P_{Y|x}}(f_1 \otimes f_2)\|_\mathcal{H} = \|f_1 \otimes \mathcal{C}_{Y|X} f_2\|_\mathcal{H}
\]
\[
= \|f_1\|_{\mathcal{H}_X} \|\mathcal{C}_{Y|X} f_2\|_{\mathcal{H}_Y}
\]
\[
\leq \|f_1\|_{\mathcal{H}_X} \|f_2\|_{\mathcal{H}_X} \|\mathcal{C}_{Y|X}\|_o
\]
\[
= \|f_1 \otimes f_2\|_o \|\mathcal{C}_{Y|X}\|_o
\]
showing that
\[
\|\tilde{\mathcal{C}}_{P_{Y|x}}\|_o \leq \|\mathcal{C}_{Y|X}\|_o < \infty.
\]
where the last inequality holds by assumption.

Next, remark that for every \( f \in \mathcal{H}_X \) the linear operator \( (f \otimes \cdot) : \mathcal{H}_Y \to \mathcal{H} \) is such that
\[
\|f \otimes \cdot\|_o \leq \|f\|_{\mathcal{H}_X} < \infty.
\]
since \[ \|f \otimes g\|_H = \|f\|_{H_X}\|g\|_{H_Y}, \quad \forall f \in H_X, \forall g \in H_Y. \]

Let \( \tilde{\mu}(P_X) = \mathbb{E}_{X \sim P_X} [k_X(X, \cdot) \otimes k_Y(Y, \cdot)] \) be the embedding of \( P_X \in \mathcal{P}(X) \) in \( H_X \otimes H_Y \). Then, for \( P'_X \in \mathcal{P}(X) \) and using the shorthand \( P' = P'_X P_Y \), we have

\[
\mu(P') = \mathbb{E}_{(X,Y) \sim P'} [k_X(X, \cdot) \otimes k_Y(Y, \cdot)] = \mathbb{E}_{X \sim P'_X} \left[ k_Y(Y, \cdot) \mathbb{E}_{Y \sim P_Y} [k_X(X, \cdot)] \right] = \mathbb{E}_{X \sim P'_X} \left[ k_X(X, \cdot) \otimes \mu(P_Y) \right] = \mathbb{E}_{X \sim P'_X} \left[ k_X(X, \cdot) \otimes C_{Y \mid X} k_X(X, \cdot) \right] = \tilde{C}_{P_Y \mid X} \mathbb{E}_{X \sim P'_X} [k_X(X, \cdot) \otimes k_X(X, \cdot)] = \tilde{C}_{P_Y \mid X} \tilde{\mu}(P_X)
\]

where the interchange between expectation and tensor product between the second and the third equality is justified by Lemma 5 and by (36), where the interchanges between expectation and tensor product between the fifth and the sixth equality is justified by Lemma 5 and by (35), while the fifth equality holds by (34).

Similarly, for \( P''_X \in \mathcal{P}(X) \) and with \( P'' = P''_X P_Y \), we have

\[
\mu(P'') = \mathbb{E}_{(X,Y) \sim P''} [k_X(X, \cdot) \otimes k_Y(Y, \cdot)]\tilde{C}_{P_Y \mid X} \tilde{\mu}(P''_X)
\]

and thus,

\[
\mathbb{D}_k(P', P'') = \|\mu(P') - \mu(P'')\|_H = \left\| \tilde{C}_{P_Y \mid X} \left( \tilde{\mu}(P_X) - \tilde{\mu}(P''_X) \right) \right\|_H \leq \left\| \tilde{C}_{P_Y \mid X} \right\|_o \|\mu(P_X) - \mu(P''_X)\|_{H_X \otimes H_Y} \leq \|C_{Y \mid X}\|_o \mathbb{D}_{k}^2(P'_X, P''_X) \tag{37}
\]

where the last inequality holds by (35). The proof is complete.

\[\square\]

### H. Proof of Lemma 3

#### H.1. Preliminary results

The following lemma is adapted from Lemma 5 in Chérief-Abdellatif and Alquier (2020). While the proof is quite similar, the statement is more general.
Lemma 10. Let $S$ be a set (equipped with a $\sigma$-algebra). Let $K$ be any symmetric function $S^2 \rightarrow [-1,1]$ that can be written $K(s,s') = \langle \varphi(s), \varphi(s') \rangle_H$ for some Hilbert space $H$ and some function $\varphi$ (note that we do not assume that $K$ is a characteristic kernel). Let $S_1, \ldots, S_n$ be independent random variables on $S$ with respective distributions $Q_1, \ldots, Q_n$. Define $Q = (1/n) \sum_{i=1}^n Q_i$ and $\hat{Q} = (1/n) \sum_{i=1}^n \delta_{S_i}$. We define, for any $Q$ and $Q'$ probability distributions on $S$,\[ D_K^2(Q,Q') = E_{S \sim Q,S' \sim Q'}[K(Z,Z')] - 2E_{S \sim Q,S' \sim Q'}[K(Z,Z')] + E_{S \sim Q',S' \sim Q'}[K(Z,Z')] \]

(which is indeed a metric if $K$ is a characteristic kernel). We have:\[ E \left[ D_K(Q,\hat{Q}) \right] \leq \frac{1}{\sqrt{n}} \text{ and } E \left[ D_K^2(Q,\hat{Q}) \right] \leq \frac{1}{n}. \]

Proof. Jensen’s inequality gives $E[D_K(Q,\hat{Q})] \leq \sqrt{E[D_K^2(Q,\hat{Q})]}$. Put $m_i = E_{S \sim Q_i}[\varphi(S)]$, then \[
E \left[ D_K^2(Q,\hat{Q}) \right] = E \left[ \left\| \frac{1}{n} \sum_{i=1}^n [\varphi(S_i) - m_i] \right\|_H^2 \right] 
\begin{align*}
&= \frac{1}{n^2} \sum_{i=1}^n E \left[ \left\| \varphi(S_i) - m_i \right\|_H^2 \right] + \frac{1}{n(n-1)} \sum_{i \neq j} E \left[ \langle \varphi(S_i) - m_i, \varphi(S_j) - m_j \rangle_H \right] \\
&= \frac{1}{n^2} \sum_{i=1}^n \left( E \left[ \left\| \varphi(S_i) \right\|_H^2 \right] - \left\| m_i \right\|_H^2 \right) + 0 \\
&\leq \frac{1}{n^2} \sum_{i=1}^n E \left[ \left\| \varphi(S_i) \right\|_H^2 \right] = \frac{1}{n^2} \sum_{i=1}^n K(S_i, S_i) \leq \frac{1}{n}. 
\end{align*} \]

\[ \square \]

Our proof strategy to study $\hat{\theta}_n(D_n)$ actually relies on the fact that despite contamination, the performance of $\hat{\theta}_n(D_n)$ remains close to the one of $\hat{\theta}_n(D_n)$. The following lemma will help to formalize this claim.

Lemma 11. Let $\hat{P}^{n,0} = \frac{1}{n} \sum_{i=1}^n \delta_{(X_i^n,Y_i^n)}$ be the non-contaminated empirical distribution and $\hat{P}^{n,0}_\theta = \frac{1}{n} \sum_{i=1}^n \delta_{X_i^n} P_\theta(\theta, X_i^n)$ be the uncontaminated counterpart of $\hat{P}_\theta^n$. Then, for any probability distribution $Q$ on $X \times Y$, we have\[ |D_k(\hat{P}^{n,0}, Q) - D_k(\hat{P}^{n}, Q)| < 2\epsilon \] (38)and\[ |D_k(\hat{P}^{n,0}_\theta, Q) - D_k(\hat{P}^{n}_\theta, Q)| < 2\epsilon. \] (39)
Proof. For the first inequality (38),
\[
\left| \mathbb{D}_k \left( \hat{P}^{n,0}, Q \right) - \mathbb{D}_k \left( \hat{P}^n, Q \right) \right| \leq \mathbb{D}_k \left( \hat{P}^{n,0}, \hat{P}^n \right) \\
= \left\| \frac{1}{n} \sum_{i=1}^{n} \left[ k((X_i^0, Y_i^0), \cdot) - k((X_i, Y_i), \cdot) \right] \right\|_H \\
\leq \frac{1}{n} \sum_{i=1}^{n} \left\| k((X_i^0, Y_i^0), \cdot) - k((X_i, Y_i), \cdot) \right\|_H \\
= \frac{1}{n} \sum_{i \in I} \left\| k((X_i^0, Y_i^0), \cdot) - k((X_i, Y_i), \cdot) \right\|_H \\
\leq \frac{1}{n} \sum_{i \in I} 2 \frac{|I|}{n} \leq 2 \epsilon.
\]

The proof of (11) is exactly the same.

H.2. Proof of the lemma

Proof. Thanks to (38) of Lemma 11, we have, for any fixed \( \theta \in \Theta \),
\[
\mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \leq \mathbb{D}_k(\hat{P}^n, \hat{P}^n) + \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \quad \text{(triangle inequality)} \\
\leq \mathbb{D}_k(\hat{P}^n, \hat{P}^n) + \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + 2 \epsilon \quad \text{where we used (38) with } Q = \hat{P}^0_n \\
\leq \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + 2 \epsilon \quad \text{by definition of } \hat{\theta}_n \\
\leq \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + 4 \epsilon \quad \text{by (38) with } Q = \hat{P}^n \\
\leq \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + 2 \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + 4 \epsilon \quad \text{(triangle inequality).}
\]

(40)

Taking the expectation in (40) gives:
\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \right] \leq 4 \epsilon + \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \right] + 2 \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \right].
\]

(41)

We can control the expectation in the right-hand side by an application of Lemma 10, where
\[
S_i = (X_i^0, Y_i^0) \sim Q_i := \delta_{X_i^0} P_{Y|X_i^0} \quad \text{that are indeed independent, and where } K = k.
\]

The lemma gives:
\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \right] \leq \frac{1}{\sqrt{n}}.
\]

(42)

We take the infimum with respect to \( \theta \) to obtain:
\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) \right] \leq 4 \epsilon + \inf_{\hat{\theta} \in \Theta} \mathbb{D}_k(\hat{P}^n, \hat{P}^0_n) + \frac{2}{\sqrt{n}}.
\]

(43)

In order to prove (11), take any \( z_i' \in Z \) and define
\[
\hat{P}^{n,0}_{(i)} = \frac{1}{n} \left( \sum_{j \neq i} \delta_{(X_j^0, Y_j^0)} + \delta_{z_i'} \right).
\]

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We note that:
\[
\left| \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}_n^0) - \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}^{\ell(n)}_n) \right| \leq \mathbb{D}_k(\hat{P}^{n,0}, \hat{P}^{\ell(n)}_n) \leq \frac{2}{n}.
\]
This allows to use the McDiarmid’s bounded difference inequality [McDiarmid (1989)], which gives:
\[
P\left\{ \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}_n^0) - \mathbb{E}\left[ \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}_n^0) \right] \geq t \right\} \leq \exp\left(-\frac{nt^2}{2}\right), \quad \forall t > 0. \quad (44)
\]
Put \( \eta = \exp(-nt^2/2) \) to get
\[
P\left\{ \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}_n^0) - \mathbb{E}\left[ \mathbb{D}_k(\hat{P}^{n,0}, \overline{P}_n^0) \right] \geq \sqrt{\frac{2\log(1/\eta)}{n}} \right\} \leq \eta,
\]
which, together with (41)-(42), gives the statement of the theorem.

\[ \square \]

I. Proof of Theorem 2

I.1. Preliminary result

**Lemma 12.** Let \( \|\cdot\| \) be a semi-norm on \( \Theta \). Let \( M : \Theta \rightarrow [0, 2] \) be such that there exists a unique \( \theta_\star \in \Theta \) verifying
\[
\inf_{\theta \in \Theta} M(\theta) = M(\theta_\star)
\]
and such that there exists a neighborhood \( U \) of \( \theta_\star \) and a constant \( \mu > 0 \) for which
\[
M(\theta) - M(\theta_\star) \geq \mu \|\theta - \theta_\star\|, \quad \forall \theta \in U.
\]
Let \( (\hat{\theta}_n)_{n \geq 1} \) be a sequence of random variables taking values in \( \Theta \) and such that there exist a strictly increasing function \( h_1 : (0, \infty) \rightarrow (0, \infty) \) with \( \lim_{x \rightarrow \infty} h_1(x) = \infty \), a continuous and strictly decreasing function \( h_2 : (0, 1) \rightarrow (0, \infty) \), and a constant \( x \geq 0 \) such that
\[
P\left\{ M(\hat{\theta}_n) < M(\theta_\star) + x + \frac{h_2(\eta)}{h_1(n)} \right\} \geq 1 - \eta, \quad \forall \eta \in (0, 1), \quad \forall n \geq 1. \quad (45)
\]
Then for any \( t > 0 \),
\[
P\left\{ \|\hat{\theta}_n - \theta_\star\| \geq x/\mu + t \right\} \leq 2h_2^{-1}\left((\mu t) \wedge (\alpha - x)_+ h_1(n)\right),
\]
and
\[
P\left\{ \|\hat{\theta}_n - \theta_\star\| < \frac{x}{\mu} + \frac{h_2(\eta)}{\mu h_1(n)} \right\} \geq 1 - \eta, \quad \forall n \geq 1, \quad \forall \eta \in \left[2h_2^{-1}((\alpha - x)_+ h_1(n)), 1\right)
\]
where \( \alpha = \inf_{\theta \in U} M(\theta) - M(\theta_\star) \in (0, 2] \).

**Remark 6.** It would also be possible to get a result on \( \mathbb{E}[\|\hat{\theta}_n - \theta_\star\|] \), but at the price of the additional assumption that the parameter space \( \Theta \) is bounded: \( \sup_{(\theta, \theta') \in \Theta^2} \|\theta - \theta'\|_\Theta < \infty \).
Proof. Note that \((45)\) is equivalent to
\[
\mathbb{P}\left\{ M(\hat{\theta}_n) - M(\theta_*) - x > t \right\} \leq h_2^{-1}(th_1(n)), \quad \forall t > 0, \quad \forall n \geq 1. \tag{46}
\]

Remind that \(\alpha = \inf_{\theta \in U^c} M(\theta) - M(\theta_*)\). It is immediate to see that \(\alpha \leq 2\). Moreover, \(\alpha > 0\), otherwise, \(U^c\) being a closed set, there would be a \(\theta' \in U^c\) such that \(M(\theta') - M(\theta_*) = 0\).

Now, for any \(t > 0\),
\[
\mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| \geq t + x/\mu \right\} = \mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| \geq t + x/\mu, \hat{\theta}_n \in U \right\} + \mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| \geq t + x/\mu, \hat{\theta}_n \notin U \right\} \\
\leq \mathbb{P}\left\{ M(\hat{\theta}) - M(\theta_*) \geq \mu t + x, \hat{\theta}_n \in U \right\} + \mathbb{P}\left\{ \hat{\theta}_n \notin U \right\} \\
\leq \mathbb{P}\left\{ M(\hat{\theta}) - M(\theta_*) \geq \mu t + x \right\} + \mathbb{P}\left\{ M(\hat{\theta}) - M(\theta_*) \geq \alpha \right\} \\
\leq h_2^{-1}(\mu t h_1(n)) + h_2^{-1}((\alpha - x)_+ h_1(n))
\]
where we used \((10)\) for the last inequality. As \(h_2^{-1}\) is strictly decreasing, we obtain:
\[
\mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| \geq t + x/\mu \right\} \leq 2h_2^{-1}[(\mu t) \wedge (\alpha - x)_+ h_1(n)] \tag{47}
\]

Fix \(\eta \in [2h_2^{-1}((\alpha - x)_+ h_1(n)), 1)\) as in the statement of the lemma, and note that
\[
2h_2^{-1}[(\mu t) \wedge (\alpha - x)_+ h_1(n)] = \eta \leftrightarrow t = \frac{h_2\left(\frac{\eta}{\mu}\right)}{\mu h_1(n)}.
\]
Plugging these values in \((47)\), we obtain:
\[
\mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| < \frac{\eta}{\mu} \right\} \geq 1 - \eta.
\]

\hfill \Box

1.2. Proof of the theorem

Proof. From Lemma \((3)\), \((15)\) in Lemma \((12)\) holds with \(\theta_* = \theta_0, x = 4\epsilon, h_1(n) = \sqrt{n}, h_2(\eta) = 2 + 2\sqrt{\log(1/\eta)}\) and \(\hat{\theta}_n = \hat{\theta}_n\). Apply Lemma \((12)\) to get:
\[
\sum_{n \geq 1} \mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| \geq 4\epsilon/\mu + t \right\} \leq 2 \sum_{n \geq 1} \exp\left[-\frac{((\mu t) \wedge (\alpha - x)_+ \sqrt{n} - 2)^2}{2}\right] < \infty, \quad \forall t > 0
\]
showing that \(\mathbb{P}\left(\limsup_{n \to \infty} \|\hat{\theta}_n - \theta_*\| \leq 4\epsilon/\mu \right) = 1\). Lemma \((12)\) also states
\[
\mathbb{P}\left\{ \|\hat{\theta}_n - \theta_*\| < \frac{h_2\left(\frac{\eta}{\mu}\right)}{\mu h_1(n)} \right\} \geq 1 - \eta, \quad \forall n \geq 1, \quad \forall \eta \in [2h_2^{-1}((\alpha - x)_+ h_1(n)), 1)\).
\]
Note that
\[
\frac{h_2\left(\frac{\eta}{\mu}\right)}{\mu h_1(n)} = \frac{1}{\mu \sqrt{n}} \left(2 + 2\sqrt{2\log(2/\eta)}\right)
\]

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and \(2h_2^{-1}((\alpha - x)_+ h_1(n)) = 2\exp(-(\alpha - x)_+ \sqrt{n} - 2)^2/2\). For the sake of simplicity, we only consider \(n \geq 16/(\alpha - x)_{+}^2\), in this case, we have \((\alpha - x)_+ \sqrt{n} - 2 \geq (\alpha - x)_{+} \sqrt{n}/2\) and thus the result holds in particular for any \(\eta \in [2\exp(-\alpha x_{+}^2/8), 1)\). Finally, remind that \(x = 4\epsilon < \alpha/8\) so it holds in particular for \(n \geq 64/\alpha^2\) and \(\eta \in [2\exp(-\alpha^2/32), 1)\).

\[\hfill\]  

\section*{J. Proof of Lemma \[4\]}

\subsection*{J.1. Preliminary result}

We start with a result that will be an essential tool in the proof of Lemma \[4\]. Essentially, it quantifies how well \(\hat{P}_{\theta_n}^{n,0} = (1/n) \sum_{i=1}^{n} \delta_{X_i} P_{\theta_n, X_i^0}\) approximates \(P^0\). Usually, in regression literature, we focus mostly on the estimation of the distribution of \(Y|X\) rather than on the estimation of the distribution of the pair \((X, Y)\). Still, we believe that this result has in interpretation on its own, so we state it as a theorem.

\textbf{Theorem 5.} Under Assumption \[4\]\footnote{\[4\]} we have

\[E \left[ D_k(\hat{P}_{\theta_n}^{n,0}, P^0) \right] \leq 8\epsilon + \inf_{\theta \in \Theta} D_k(P_\theta, P^0) + \frac{3}{\sqrt{n}} \]  

and, for any \(\eta \in (0, 1)\),

\[P \left\{ D_k(\hat{P}_{\theta_n}^{n,0}, P^0) \leq 8\epsilon + \inf_{\theta \in \Theta} D_k(P_\theta, P^0) + \frac{3}{\sqrt{n}} \left( 1 + \sqrt{2\log(2/\eta)} \right) \} \geq 1 - \eta. \]

\textit{Proof.} The proof is quite similar to the proof of Lemma \[3\] but requires some adaptations, in particular in the application of Lemma \[10\].

First,  

\[D_k(\hat{P}_{\theta_n}^{n,0}, P^0) \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n,0}) + D_k(\hat{P}^{n,0}, P^0). \]  \hfill (48)

Let us deal with the first term of this upper bound in a first time. Here, we will use both \(38\) and \(39\) of Lemma \[11\]. We have:

\[D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n,0}) \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n}) + 2\epsilon \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n}) + 4\epsilon \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n}) + 4\epsilon \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n}) + 4\epsilon \leq D_k(\hat{P}_{\theta_n}^{n,0}, \hat{P}^{n}) + 4\epsilon. \]

where the first inequality uses \(38\), the second \(39\), the third the definition of \(\hat{\theta}_n\), the fourth \(39\), the fifth \(38\) and the sixth the definition of \(\hat{\theta}_n\).
Together with (48), this shows that
\[
\mathbb{D}_k(\hat{P}^{n,0}, P^0) \leq \inf_{\theta \in \Theta} \mathbb{D}_k(\hat{P}^{n,0}, P^0) + \inf_{\theta \in \Theta} \mathbb{D}_k(P^{n,0}, P^0) + 8\epsilon \\
\leq \inf_{\theta \in \Theta} \mathbb{D}_k(\hat{P}^{n,0}, P^0) + 2\mathbb{D}_k(P^{n,0}, P^0) + 8\epsilon \\
\leq \inf_{\theta \in \Theta} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) + \mathbb{D}_k(P^0, P^0) \right] + 2\mathbb{D}_k(\hat{P}^{n,0}, P^0) + 8\epsilon 
\]
and so, taking expectations on both sides,
\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right] \leq \inf_{\theta \in \Theta} \left\{ \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right] + \mathbb{D}_k(P^0, P^0) \right\} 2\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right] + 8\epsilon.
\]

We tackle the term \( \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right] \). Letting \( \Phi \) denote the function such that \( k((x, y), (x', y')) = \langle \Phi(x, y), \Phi(x', y') \rangle_{\mathcal{H}} \), we have
\[
\mathbb{D}_k(\hat{P}^{n,0}, P^0) = \sqrt{\mathbb{D}_k^2(\hat{P}^{n,0}, P^0)}
\]
\[
= \left( \mathbb{E}_{(X,Y) \sim \hat{P}^{n,0}} \langle \Phi(X,Y), \Phi(X',Y') \rangle_{\mathcal{H}} + 2\mathbb{E}_{(X,Y) \sim \hat{P}^{n,0}} \langle \Phi(X,Y), \Phi(X',Y') \rangle_{\mathcal{H}} \right)^{\frac{1}{2}}
\]
\[
= \left( \mathbb{E}_{X \sim \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}} \mathbb{E}_{Y \sim \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}} \langle \mathbb{E}_{Y \sim P_g(\theta,X)} [\Phi(X,Y)], \mathbb{E}_{Y' \sim P_g(\theta,X)} [\Phi(X,Y')] \rangle_{\mathcal{H}} + 2\mathbb{E}_{X \sim \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}} \mathbb{E}_{Y' \sim \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}} \langle \mathbb{E}_{Y \sim P_g(\theta,X)} [\Phi(X,Y)], \mathbb{E}_{Y' \sim P_g(\theta,X)} [\Phi(X,Y')] \rangle_{\mathcal{H}} \right)^{\frac{1}{2}}
\]
\[
= \left( \mathbb{D}_k^2 \left( \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}, P^0_X \right) \right)^{\frac{1}{2}}
\]
where the function \( \tilde{k} \) is given by:
\[
\tilde{k}(x, x') = \langle \mathbb{E}_{Y \sim P_g(\theta,x)} [\Phi(x,Y)], \mathbb{E}_{Y' \sim P_g(\theta,x')} [\Phi(x',Y')] \rangle_{\mathcal{H}}.
\]
Note that \(-1 \leq \tilde{k} \leq 1\) so we can apply Lemma 10 to \( S_i = X_i^0 \sim Q_i = P^0_X \) and \( K = \tilde{k} \) to get:
\[
\mathbb{E} \left[ \mathbb{D}_{\tilde{k}} \left( \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}, P^0_X \right) \right] \leq \frac{1}{\sqrt{n}}.
\]
Combining this last result with (50), and applying Lemma 10 with \( S_i = (X_i^0, Y_i^0) \sim Q_i = P^0 \) and \( K = k \) that gives \( \mathbb{E}[\mathbb{D}_k(P^{n,0}, P^0)] \leq 1/\sqrt{n} \), we finally obtain:

\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}_{\theta_n}, P^0) \right] \leq \inf_{\theta \in \Theta} \left\{ \frac{1}{\sqrt{n}} + \mathbb{D}_k(P_\theta, P^0) \right\} + \frac{2}{\sqrt{n}} + 8\epsilon
\]

\[
= \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) + \frac{3}{\sqrt{n}} + 8\epsilon,
\]

that is the first inequality of the theorem.

In order to prove the second inequality let \( \theta_0 \in \arg\min_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) \). Then (49) implies

\[
\mathbb{D}_k(\hat{P}^{n,0}_{\theta_n}, P^0)
\]

\[
\leq \mathbb{D}_k(\hat{P}^{n,0}_{\theta_0}, P_{\theta_0}) + \mathbb{D}_k(P_{\theta_0}, P^0) + 2\mathbb{D}_k(\hat{P}^{n,0}_{\theta_0}, P^0) + 8\epsilon
\]

\[
= \mathbb{D}_k(\hat{P}^{n,0}_{\theta_0}, P_{\theta_0}) + \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) + 2\mathbb{D}_k(\hat{P}^{n,0}_{\theta_0}, P^0) + 8\epsilon.
\]

McDiarmid’s bounded difference inequality leads to

\[
P \left\{ \mathbb{D}_k(\hat{P}^{n,0}, P^0) - \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right] \geq t \right\} \leq \exp \left( -\frac{nt^2}{2} \right)
\]

and to

\[
P \left\{ \mathbb{D}_k(\hat{P}^{n,0}, P^0) - \mathbb{E} \left( \mathbb{D}_k(\hat{P}^{n,0}, P^0) \right) \geq t \right\} \leq \exp \left( -\frac{nt^2}{2} \right).
\]

By a union bound, the probability that one of the two events hold is smaller or equal to \( 2 \exp(\frac{-nt^2}{2}) \), which leads to

\[
P \left\{ \mathbb{D}_k(\hat{P}^{n,0}_{\theta_n}, P^0) \leq \inf_{\theta \in \Theta} \mathbb{D}_k(P_\theta, P^0) + \frac{3}{\sqrt{n}} \left( 1 + \sqrt{2 \log(2/\eta)} \right) + 8\epsilon \right\} \geq 1 - \eta.
\]

This ends the proof.

\[
\square
\]

J.2. Proof of the lemma

Proof. By Lemma 2 applied to \( P_X = \hat{P}^{n,0}_X \) and \( P''_X = P^0_X \), we have

\[
\mathbb{D}_k(\hat{P}^{n}_{\theta_n, P_{\theta_n}}) \leq \mathcal{C} \mathbb{D}_k(\hat{P}^{n,0}_X, P^0_X)
\]

and thus

\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}_{\theta_n, P_{\theta_n}}) \right] \leq \mathcal{C} \mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}_X, P^0_X) \right].
\]

Applying Lemma 10 with \( Z_i = X_i \sim Q_i = P^0 \) and \( K = k^2_X \), we obtain

\[
\mathbb{E} \left[ \mathbb{D}_k(\hat{P}^{n,0}_{\theta_n, P_{\theta_n}}) \right] \leq \frac{\mathcal{C}}{\sqrt{n}}.
\]
Now:

\[
E \left[ \mathcal{D}_k(P_{\hat{\theta}_n}, P^0) \right] \leq E \left[ \mathcal{D}_k(P_{\hat{\theta}_n}, \hat{P}_{\hat{\theta}_n}) \right] + E \left[ \mathcal{D}_k(\hat{P}_{\hat{\theta}_n}, P^0) \right] \\
\leq \frac{\epsilon}{\sqrt{n}} + \left( \inf_{\theta \in \Theta} \mathcal{D}_k(P_{\theta}, P^0) + 8\epsilon + \frac{3}{\sqrt{n}} \right)
\]

where we used (52) to upper bound the first term, and Theorem 5 for the second term. This ends the proof of the bound in expectation.

Let us now prove the inequality in probability. Let \( \eta \in (0,1) \) and use the bounded difference inequality to get

\[
P \left\{ \mathcal{D}_k(\hat{P}_{\hat{\theta}_n}, P^0) \leq 8\epsilon + \inf_{\theta \in \Theta} \mathcal{D}_k(P_{\theta}, P^0) + \frac{3}{\sqrt{n}} \right(1 + \sqrt{2 \log(4/\eta)}\right) \right\} \leq 1 - \frac{\eta}{2}
\]

while, by Theorem 5

\[
P \left\{ \mathcal{D}_k(\hat{P}_{\hat{\theta}_n}, P^0) \leq 8\epsilon + \inf_{\theta \in \Theta} \mathcal{D}_k(P_{\theta}, P^0) + \frac{3}{\sqrt{n}} \right(1 + \sqrt{2 \log(4/\eta)}\right) \right\} \leq 1 - \frac{\eta}{2}
\]

Together with (51), and using a union bound, we obtain

\[
P \left\{ \mathcal{D}_k(P_{\hat{\theta}_n}, P^0) \leq \inf_{\theta \in \Theta} \mathcal{D}_k(P_{\theta}, P^0) + \frac{3(1 + \sqrt{2 \log(4/\eta)}) + \epsilon(1 + \sqrt{2 \log(2/\eta)})}{\sqrt{n}} \right\} \\
\geq 1 - \eta.
\]

\[\square\]

K. Proof of Theorem 3

Proof. From Lemma 11 (15) in Lemma 12 holds with \( h_1(n) = \sqrt{n}, h_2(\eta) = (\epsilon + 3)(1 + \sqrt{2 \log(4/\eta)}) \) and \( \hat{\theta}_n = \hat{\theta}_n \). Then, the result is proved following the computations done in the proof of Theorem 2

\[\square\]

L. Proof of Proposition 2

Proof. Let \( f : \Theta \rightarrow [0,4] \) be defined by

\[
f(\theta) = (\mathcal{D}_k(P_{\theta}, \hat{P}^0) - \mathcal{D}_k(P_{\bar{\theta}_n}, \hat{P}^0))^2, \quad \theta \in \Theta
\]

and let \( U \) be an open set containing \( \theta_0 \) such that \( f \) is twice continuously differentiable on \( U \). Let \( H_{\hat{\theta}} \) be the Hessian matrix of \( f \) evaluated at \( \theta \in U \).
Then, using Taylor’s theorem, for every \( \theta \in U \) we have, for some \( \tau \in [0, 1] \)

\[
f(\theta) = f(\theta_0) + (\theta - \theta_0)^\top \nabla f(\theta_0) + \frac{1}{2}(\theta - \theta_0)^\top H_{\theta_0 + \tau(\theta - \theta_0)}(\theta - \theta_0)
\]

\[
= (\theta - \theta_0)^\top H_{\theta_0 + \tau(\theta - \theta_0)}(\theta - \theta_0)
\]

\[
\geq \|\theta - \theta_0\|^2 \frac{\lambda_{\text{min}}(H_{\theta_0 + \tau(\theta - \theta_0)})}{2}
\]

\[
\geq \|\theta - \theta_0\|^2 \inf_{\theta \in U, \tau \in [0, 1]} \frac{\lambda_{\text{min}}(H_{\theta_0 + \tau(\theta - \theta_0)})}{2}
\]

where for every \( \theta \in U \) we denote by \( \lambda_{\text{min}}(H_\theta) \) the minimum eigenvalue of \( H_\theta \). Under the assumptions of the proposition, we can take \( U \) sufficiency small so that \( c := \inf_{\theta \in U, \tau \in [0, 1]} \lambda_{\text{min}}(H_{\theta_0 + \tau(\theta - \theta_0)}) > 0 \). Then,

\[
\mathbb{D}_k(P_\theta, \tilde{P}_0) - \mathbb{D}_k(P_{\hat{\theta}}, \tilde{P}_0) = \sqrt{\hat{f}(\theta)} \geq \sqrt{c/2} \|\theta - \theta_0\|
\]

showing that (14) holds for \( \mu = \sqrt{c/2} \).

\[\square\]

M. Proof of Proposition 3

Proof. For all \( (\theta, x, y) \in \Theta \times \mathcal{X} \times \mathcal{Y} \), let

\[
m_\theta(x, y) = \mathbb{E}_{Y \sim P_{g(\theta, x)}} [\kappa_y(Y, Y')] - 2\kappa_y(Y, y) + \mathbb{E}_{X \sim P_0^X} \left[ \mathbb{E}_{Y \sim P_{g(\theta, X)}} [\kappa_y(Y, Y')] \right]
\]

and remark that

\[
\mathbb{E}_{(X, Y) \sim P_0} [m_\theta(X, Y)] = \mathbb{E}_{X \sim P_0^X} \left[ \mathbb{D}_{k_y}(P_{g(\theta, X)}, P_{Y|X}^0)^2 \right], \quad \forall \theta \in \Theta.
\]

Under the assumptions of the theorem, the mapping \( \theta \mapsto m_\theta(x, y) \) is continuous on the compact set \( \Theta \) and is such that \( |m_\theta(x, y)| \leq 4 \) for all \( (\theta, x, y) \in \Theta \times \mathcal{X} \times \mathcal{Y} \). Then (see e.g. Van der Vaart 2000, page 46)

\[
\sup_{\theta \in \Theta} \left| \frac{1}{n} \sum_{i=1}^n m_\theta(X_i, Y_i) - \mathbb{E}_{X \sim P_0^X} \left[ \mathbb{D}_{k_y}(P_{g(\theta, X)}, P_{Y|X}^0)^2 \right] \right| \rightarrow 0, \quad \text{in } \mathbb{P}-\text{probability}
\]

and therefore, noting that \( \hat{\theta}_n \in \arg\min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n m_\theta(X_i, Y_i) \), the result follows by Van der Vaart (2000, Theorem 5.7).

\[\square\]

N. Proof of Theorem 4

Proof. Let \( \epsilon \in [0, 1) \) and, for all \( x \in \mathcal{X} \), let \( \tilde{P}_{Y|X}^0 = (1 - \epsilon)P_{Y|X}^0 + \epsilon Q_{Y|X} \) and \( \tilde{P}_X^0 = (1 - \epsilon)P_X^0 + \epsilon Q_X \) where \( Q_X \) denotes the distribution of \( X \) under \( Q \).
Then, for all $\theta \in \Theta$ we have
\[
E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},P^0_Y|X)^2 \right] \\
\leq E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X) + \mathbb{D}_{k_y}(P^0_Y|X,\tilde{P}^0_Y|X)^2 \right] \\
\leq E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X) + 2\epsilon \right]^2 \\
\leq E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + 8\epsilon + 4\epsilon^2 \\
\leq E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + 12\epsilon \\
\leq \frac{1}{1 - \epsilon} E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + 12\epsilon \\
\leq \frac{1}{1 - \epsilon} \inf_{\theta \in \Theta} E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + 12\epsilon \\
\leq \frac{1}{1 - \epsilon} \inf_{\theta \in \Theta} E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + \frac{24\epsilon}{1 - \epsilon} + \frac{12\epsilon}{1 - \epsilon} + 16\epsilon \\
\leq \frac{1}{1 - \epsilon} \inf_{\theta \in \Theta} E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] + \frac{52\epsilon}{1 - \epsilon}
\]
where the third inequality follows by swapping $\tilde{P}^0_Y$ and $P^0_Y|X$ in \((53)\) and the third one uses the fact that, since $|k_Y| \leq 1,

\begin{align*}
E_{X \sim Q_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] &\leq 4, \quad \forall \theta \in \Theta.
\end{align*}

By assumption, $\tilde{\theta}_0$ is the unique minimizer of the function $\theta \mapsto E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right]$ and therefore (see the proof of Lemma \([12]\))
\[
\alpha = \inf_{\theta \in U} \left( E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},P^0_Y|X)^2 \right] - E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\tilde{\theta}_0,X)},P^0_Y|X)^2 \right] \right) > 0.
\]
Together with \([54]\), this shows that if
\[
\frac{52\epsilon}{1 - \epsilon} < \alpha \iff \epsilon < \frac{\alpha}{52 + \alpha}
\]
then
\[
E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta_0,X)},\tilde{P}^0_Y|X)^2 \right] - E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\tilde{\theta}_0,X)},\tilde{P}^0_Y|X)^2 \right] \\
< \inf_{\theta \in U} \left( E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\theta,X)},\tilde{P}^0_Y|X)^2 \right] - E_{X \sim P^0_X} \left[ \mathbb{D}_{k_y}(P_{g(\tilde{\theta}_0,X)},\tilde{P}^0_Y|X)^2 \right] \right)
\]
implying that $\hat{\theta}_{Q, \epsilon} \in U$. Consequently, using again \((54)\),

$$\frac{5\epsilon}{1 - \epsilon} \geq \mathbb{E}_{X \sim P_X} \left[ \mathbb{D}_{k_{2}} \left( P_{g(\hat{\theta}_{Q, \epsilon}, X)}; P_{0|X} \right) \right] - \mathbb{E}_{X \sim P_X} \left[ \mathbb{D}_{k_{2}} \left( P_{g(\hat{\theta}_{0}, X)}; P_{0|X} \right) \right] \geq \mu \| \hat{\theta}_{Q, \epsilon} - \theta_0 \|
$$

and the result follows. \qed