Robust learning with the Hilbert-Schmidt independence criterion

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Abstract

We investigate the use of a non-parametric independence measure, the Hilbert-Schmidt Independence Criterion (HSIC), as a loss-function for learning robust regression and classification models. This loss-function encourages learning models where the distribution of the residuals between the label and the model-prediction is statistically independent of the distribution of the instances themselves. This loss-function was first proposed by Mooij et al. [15] in the context of learning causal graphs. We adapt it to the task of robust learning for unsupervised covariate shift: learning on a source domain without access to any instances or labels from the unknown target domain. We prove that the proposed loss is expected to generalize to a class of target domains described in terms of the complexity of their density ratio function with respect to the source domain. Experiments on tasks of unsupervised covariate shift demonstrate that models learned with the proposed loss-function outperform several baseline methods.

1 Introduction

In recent years there has been much interest in methods for learning robust models: models that are learned using certain data but perform well even on data which is drawn from a distribution which is different from the training distribution. This interest stems from several sources: One is the realization that many modern learning systems, especially deep-learning based systems, are subject to adversarial attacks that can severely compromise their performance [? ]. Another is the demand for models which can perform under conditions of transfer learning and domain adaptation [? ]. This is especially relevant in domains where training datasets are collected in a process which is artificial to some degree, such as image collections. These training sets are often restricted to a certain time and place, while the learned models are expected to generalize to cases which are beyond the specifics of how the training data was collected.

More specifically, we consider the following learning problem, called unsupervised covariate shift. Let \((X, Y)\) be a pair of random variables such that \(X \in \mathcal{X}\) and \(Y \in \mathcal{Y} \subseteq \mathbb{R}\), with a joint distribution \(P(X, Y)\). We consider \(X\) as the instances and \(Y\) as the labels, where the task is to predict \(Y\) when we are given \(X\). In a covariate shift scenario, \(P(Y \mid X)\) remains the same during test time, but the marginal distribution \(P(X)\) can change. We focus on unsupervised covariate shift, where we have no access to samples \(X\) or \(Y\) from the target domain.

In this paper we propose using a loss function inspired by work in the causal inference community. We consider a model in which the relation between the instance \(X\) and its label \(Y\) is of the form:

\[
Y = f^*(X) + \epsilon, \quad \epsilon \perp \! \! \! \perp X,
\]

where the variable \(\epsilon\) denotes noise which is independent of the distribution of the random variable \(X\). Given a well-specified model family and enough samples, one can learn \(f^*\), in which case there is no need to worry about covariate shift. However, in many realistic cases we cannot expect to have the

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true model in our model class, nor can we expect to have enough samples to learn the true model even if it is in our model class. Thus, in cases of small sample size or model mis-specification, there is room to study objective functions that are robust to covariate shift. Throughout this work we do not assume that the model is well-specified, nor that we have any samples from a test distribution.

The basic idea presented in this paper is as follows: by Eq. (1) we have \( Y - f^*(X) \perp\!\!\!\perp X \). Standard loss functions aim to learn a model \( \hat{f} \) such that \( \hat{f}(X) \approx Y \), or such that \( \hat{p}(Y|X) \) is high. We follow a different approach: learning a model \( \hat{f} \) such that \( Y - \hat{f}(X) \) is approximately independent of the distribution of \( X \). Specifically, we propose measuring independence using the Hilbert Schmidt Independence Criterion (HSIC): a non-parametric method that does not assume a specific noise distribution for \( \varepsilon \) \([7, 8]\). Such an approach, in the context of causal inference, was first proposed by Mooij et al. \([15]\). As Mooij et al. \([15]\) point out, this approach can be contrasted with learning with loss functions such as the squared-loss or absolute-loss, which implicitly assume that \( \varepsilon \) has, respectively, a Gaussian or Laplacian distribution.

Intuitively, covariate shift is most detrimental when the target distribution has more mass on areas of \( \mathcal{X} \) on which the learned model performs badly. Thus, defending against the worst-case covariate shift scenario entails opting for a model that performs well across all subsets of \( \mathcal{X} \) (of positive measure). Put differently, opting for a model whose errors are independent of \( X \).

The following toy example showcases that standard loss functions do not necessarily have such properties. Suppose \( \mathcal{X} = \{0, 1\} \), and \( Y = X \). Let \( P(X = 0) = \varepsilon \), and consider the following hypothesis class: \( \mathcal{H} = \{h_1, h_2\} \), where \( h_1(x) = 1 \) for all \( x \), and \( h_2(x) = x - 0.01 \). For small values of \( \varepsilon \), an algorithm minimizing the mean squared error (or any standard loss) will output \( h_1 \). An algorithm relying on the independence criteria on the other hand will output \( h_2 \), since its residuals are independent of \( X \). Which is preferable? That depends on the target (test) distribution. If it is the same as the training distribution, \( h_1 \) is indeed a better choice. However, if we do not know the target distribution, then \( h_2 \) might be the better choice since it will always incur relatively small loss, as opposed to \( h_1 \) which might have very poor performance, say if \( P(X = 0) = 0 \) and \( P(X = 1) = 1 \) are switched during test time. While pursuing robustness against any change in \( P(X) \) is difficult, we will show below that learning with the HSIC-loss provides a natural trade-off between the generalization guarantees and the complexity of the changes in distribution.

Our contributions relative to the first proposal by Mooij et al. \([15]\) are as follows:

1. We prove that the HSIC objective is learnable for an hypothesis class of bounded Rademacher complexity.
2. We give a lower bound on the HSIC-loss in terms of the \( L_2 \) loss, up to easily estimated source distribution bias terms.
3. We prove that minimizing the HSIC-loss minimizes a worst-case loss over a class of unsupervised covariate shift tasks.
4. We provide experimental validation using both linear models and deep networks, showing that learning with the HSIC-loss is competitive on a variety of unsupervised covariate shift benchmarks. We also provide code, including a PyTorch \([17]\) class for the HSIC-loss.

2 Background and set up

A useful method for testing if two random variables are independent, introduced by Gretton et al. \([7, 8]\), is the Hilbert-Schmidt independence criterion (HSIC). We give the basics of HSIC here, following the presentation in Gretton et al. \([7, 8]\).

The root of the idea is that while \( \text{Cov}(A, B) = 0 \) does not imply that two random variables \( A \) and \( B \) are independent, having \( \text{Cov}(s(A), t(B)) = 0 \) for all bounded continuous functions \( s \) and \( t \) does actually imply independence \([18]\). Since going over all bounded continuous functions is not tractable, Gretton et al. \([6]\) propose evaluating \( \sup_{s \in F, t \in G} \text{Cov} [s(x), t(y)] \) where \( F, G \) are universal Reproducing Kernel Hilbert Spaces (RKHS). This allows for a tractable computation and is equivalent in terms of the independence property. Gretton et al. \([7]\) then introduced HSIC as an upper bound to the measure introduced by Gretton et al. \([6]\), showing it has superior performance and is easier to work with statistically and algorithmically.
2.1 RKHS background

A reproducing kernel Hilbert space $F$ is a Hilbert space of functions from $X$ to $\mathbb{R}$ with the following (reproducing) property: there exist a positive definite kernel $K : X \times X \to \mathbb{R}$ and a mapping function $\phi$ from $X$ to $F$ s.t. $K(x_1, x_2) = \langle \phi(x_1), \phi(x_2) \rangle_F$. Given two separable (having a complete orthonormal basis) RKHSs $F$ and $G$ on metric spaces $X$ and $Y$, respectively, and a linear operator $C : F \to G$, the Hilbert-Schmidt norm of $C$ is defined as follows:

$$\|C\|_{HS} = \sum_{i,j} \langle Cu_i, v_j \rangle_G^2,$$

where $\{u_i\}$ and $\{u_i\}$ are some orthonormal basis for $F$ and $G$ respectively. Here we consider two probability spaces $X$ and $Y$ and their corresponding RKHSs $F$ and $G$. The mean elements $\mu_x$ and $\mu_y$ are defined such that $\langle \mu_x, s \rangle_F := \mathbb{E}[\langle \phi(x), s \rangle_F] = \mathbb{E}[s(x)]$, and likewise for $\mu_y$. Notice that we can compute the norms of these operators quite easily: $\|\mu_x\|^2_F = \mathbb{E}[K(x_1, x_2)]$ where the expectation is done over i.i.d. samples of pairs from $X$. For $s \in F$ and $t \in G$, their tensor product $s \otimes t : G \to F$ is defined as follows: $(s \otimes t)(h) = \langle t, h \rangle_G : s$. The Hilbert-Schmidt norm of the tensor product can be shown to be given by $\|s \otimes t\|^2_{HS} = \|s\|^2_F \cdot \|t\|^2_G$. Equipped with these definitions, we are ready to define the cross covariance operator $C_{xy} : G \to F$:

$$C_{xy} = \mathbb{E}[\phi(x) \otimes \psi(y)] - \mu_x \otimes \mu_y.$$

2.2 HSIC

Consider two random variables $X$ and $Y$, residing in two metric spaces $X$ and $Y$ with a joint distribution on them, and two separable RKHSs $F$ and $G$ on $X$ and $Y$ respectively. HSIC is defined as the Hilbert-Schmidt norm of the cross covariance operator:

$$\text{HSIC}(X, Y; F, G) \equiv \|C_{xy}\|^2_{HS}.$$

Gretton et al. [7] show that:

$$\text{HSIC}(X, Y; F, G) \geq \sup_{s \in F, t \in G} \text{Cov}[s(x), t(y)],$$

an inequality which we use extensively for our results.

We now state Theorem 4 of Gretton et al. [7], which shows the properties of HSIC as an independence test:

**Theorem 1** (Gretton et al. [7], Theorem 4). Denote by $F$ and $G$ RKHSs both with universal kernels, $k$, $l$ respectively on compact domains $X$ and $Y$. Assume without loss of generality that $\|s\|_\infty \leq 1$ for all $s \in F$ and likewise $\|t\|_\infty \leq 1$ for all $t \in G$.

Then the following holds: $\|C_{xy}\|^2_{HS} = 0$ if and only if $X \perp Y$.

Let $\{(x_i, y_i)\}_{i=1}^n$ be i.i.d. samples from the joint distribution on $X \times Y$. The empirical estimate of HSIC is given by:

$$\hat{\text{HSIC}}\{(x_i, y_i)\}_{i=1}^n; F, G) = \frac{1}{(n-1)^2} \text{tr} KHLH,$$

where $K_{i,j} = k(x_i, x_j)$, $L_{i,j} = l(y_i, y_j)$ are kernel matrices for the kernels $k$ and $l$ respectively, and $H_{i,j} = \delta_{i,j} - \frac{1}{n}$ is a centering matrix. The main result of Gretton et al. [7] is that the empirical estimate HSIC converges to HSIC at a rate of $O\left(\frac{1}{n^{1/2}}\right)$, and its bias is of order $O\left(\frac{1}{n}\right)$.

3 Proposed method

Throughout this paper, we consider learning functions of the sort $Y = f^*(X) + \varepsilon$, where $X$ and $\varepsilon$ are independent random variables drawn from a distribution $D$. This presentation assumes a mechanism tying together $X$ and $Y$ through $f$, up to independent noise factors. A typical learning approach is to set some hypothesis class $\mathcal{H}$, and attempt to solve the following problem:

$$\min_{h \in \mathcal{H}} \mathbb{E}_{X, \varepsilon \sim D}[\ell(y, h(x))],$$

Often this is taken to mean that the direction of causation is “$X$ causes $Y$” [22], though below we also experiment with cases where this is not necessarily so.
where \( \ell \) is often the squared loss function in a regression setting, or the cross entropy loss in case of classification.

Here, following Mooij et al. [15], we suggest using a loss function which penalizes hypotheses whose residual from \( Y \) is not independent of the instance \( X \). Concretely, we pose the following learning problem:

\[
\min_{h \in \mathcal{H}} HSIC(X, Y - h(X); \mathcal{F}, \mathcal{G}),
\]

(4)

where we approximate the learning problem with empirical samples using \( \hat{HSIC} \) as shown in Eq. (3). Unlike typical loss functions, this loss does not decompose as a sum of losses over each individual sample. In Algorithm [1] we present a general gradient-based method for learning with this loss.

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**Algorithm 1:** Learning with HSIC-loss

**Input:** samples \( \{(x_i, y_i)\}_{i=1}^n \), kernels \( k, l \), a hypothesis \( h_\theta \) parameterized by \( \theta \), and a batch size \( m > 1 \).

1. **while** in training phase **do**
2. Sample mini-batch \( \{(x_i, y_i)\}_{i=1}^m \)
3. Compute the residuals \( r_i^\theta = y_i - h_\theta(x_i) \)
4. Compute the kernel matrices \( K_{i,j} = k(x_i, x_j) \), and \( R_{i,j}^\theta = l(r_i^\theta, r_j^\theta) \)
5. Compute the HSIC-loss on the mini-batch: \( \text{Loss}(\theta) = \text{tr}(KH\hat{R}H)/(m-1)^2 \) where \( H_{i,j} = \delta_{i,j} - \frac{1}{m} \)
6. Update: \( \theta \leftarrow \theta - \alpha \cdot \nabla \text{Loss}(\theta) \)
7. Compute the estimated source bias \( b \leftarrow \frac{1}{n} \sum_{i=1}^n y_i - \frac{1}{b} \sum_{i=1}^n h_\theta(x_i) \)

**Output:** A bias-adjusted hypothesis \( h(x) = h_\theta(x) + b \)

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As long as the kernel function \( k(,\cdot) \) and \( l(,\cdot) \) are differentiable, taking the gradient of Loss(\( \theta \)) is simple with any automatic differentiation software [17, 1]. We note that HSIC \( \text{HSIC}(X, Y - h(X); \mathcal{F}, \mathcal{G}) \) is exactly the same for any two functions \( h_1(X), h_2(X) \) who differ only by a constant. This can be seen by the examining the role of the centering matrix \( H \), or from the invariance of the covariance operator under constant shifts. Therefore, the predictor obtained from solving (4) is determined only up to a constant term. To determine the correct bias, one can infer it from the empirical mean of the observed \( Y \) values. If there is reason to believe \( \mathbb{E}[Y] \) will change in the test phase, one can try and correct the bias with some estimate of the new mean.

### 4 Theoretical results

We now prove several properties of the HSIC-loss, motivating its use as a robust loss function. We consider models of the form given in Eq. (1) such that \( \varepsilon \) has zero mean. Assume that \( X \in \mathcal{X} \) and \( Y \in \mathcal{Y} \), where \( \mathcal{X}, \mathcal{Y} \) are compact metric spaces. Denote by \( \mathcal{F} \) and \( \mathcal{G} \) reproducing kernel Hilbert spaces of functions from \( \mathcal{X} \) and \( \mathcal{Y} \) respectively, to \( \mathbb{R} \) s.t. that \( \|f\|_\mathcal{F} \leq M_\mathcal{F} \) for all \( f \in \mathcal{F} \) and \( \|g\|_\mathcal{G} \leq M_\mathcal{G} \) for all \( g \in \mathcal{G} \). We will use \( M_\mathcal{G} \) and \( M_\mathcal{F} \) throughout this section.

Denote by \( \hat{\mathcal{F}} \) and \( \hat{\mathcal{G}} \) the restriction of \( \mathcal{F} \) and \( \mathcal{G} \) to functions in the unit ball of the respective RKHS. Before we state the results, we give the following useful lemma:

**Lemma 2.** Suppose \( \mathcal{F} \) and \( \mathcal{G} \) are RKHSs over \( \mathcal{X} \) and \( \mathcal{Y} \), s.t. \( \|s\|_\mathcal{F} \leq M_\mathcal{F} \) for all \( s \in \mathcal{F} \) and \( \|t\|_\mathcal{G} \leq M_\mathcal{G} \) for all \( t \in \mathcal{G} \). Then the following holds:

\[
\sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)] = M_\mathcal{F} \cdot M_\mathcal{G} \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)].
\]

**Proof.** We prove that \( \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)] \leq M_\mathcal{F} \cdot M_\mathcal{G} \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)] \). The other direction of the inequality is true by that same arguments.

Let \( \{s_i\}_{i=1}^\infty \subset \mathcal{F} \) and \( \{t_i\}_{i=1}^\infty \subset \mathcal{G} \) be such that

\[
\lim_{n \to \infty} \text{Cov}[s(X), t_i(Y)] = \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)].
\]
Since for all \( i, \frac{1}{M_{\mathcal{F}}} s_i \in \tilde{\mathcal{F}} \) and likewise \( \frac{1}{M_{\mathcal{G}}} t_i \in \tilde{\mathcal{G}} \), we have that
\[
\sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)] = \lim_{n \to \infty} \text{Cov}[s_i(X), t_i(Y)]
\]
\[
= M_{\mathcal{F}} \cdot M_{\mathcal{G}} \lim_{n \to \infty} \text{Cov}[\frac{1}{M_{\mathcal{F}}} s_i(X), \frac{1}{M_{\mathcal{G}}} t_i(Y)]
\]
\[
\leq M_{\mathcal{F}} \cdot M_{\mathcal{G}} \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}[s(X), t(Y)].
\]

\[\square\]

4.1 Lower bound

Before exploring the robustness properties of the HSIC-loss, we relate it to standard notions of model performance. Specifically, we show that under additional mild assumptions, the HSIC-loss is an upper bound to the variance of the residual \( f^*(X) - h(X) \). The additional assumption here is that for all \( h \in \mathcal{H} \), \( f^* - h \) is in the closure of \( \mathcal{F} \), and that \( \mathcal{G} \) contains the identity function from \( \mathbb{R} \) to \( \mathbb{R} \).

This means that \( M_{\mathcal{F}} \) acts as a measure of complexity of the true function \( f^* \) that we are trying to learn.

Note however, that this does not imply that the hypothesis class \( \mathcal{H} \) is well specified, but rather that this is an assumption on the kernel space used to calculate the HSIC term.

**Theorem 3.** Under the conditions specified above, the following holds:

\[
\forall \text{Var}(f^*(X) - h(X)) \leq M_{\mathcal{F}} \cdot M_{\mathcal{G}} \cdot \text{HSIC}(X, Y - h(X); \tilde{\mathcal{F}}, \tilde{\mathcal{G}}).
\]

**Proof.** Expanding the HSIC-loss:

\[
\text{HSIC}(X, Y - h(X); \tilde{\mathcal{F}}, \tilde{\mathcal{G}}) \geq \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}(s(X), t(Y) - h(X))
\]

\[
= \frac{1}{M_{\mathcal{F}} \cdot M_{\mathcal{G}}} \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}(s(X), t(Y) - h(X))
\]

\[
= \frac{1}{M_{\mathcal{F}} \cdot M_{\mathcal{G}}} \sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}(s(X), (f^*(X) - h(X) + \varepsilon),
\]

where the first inequality is due to Eq. (2), and the first equality by Lemma[2]. Now, by the assumption that \( f^* - h \) is in the closure of \( \mathcal{F} \), there exist \( s_n \in \mathcal{F} \) s.t. \( (s_n)_{n=1} \) converge to \( f^* - h \) under the infinity norm. Taking \( t \) to be the identity function, we get that for all \( n \in \mathbb{N} \):

\[
\sup_{s \in \mathcal{F}} \text{Cov}(s(X), f^*(X) - h(X) + \varepsilon) \geq \text{Cov}(s_n(X), (f^*(X) - h(X) + \varepsilon),
\]

which implies that

\[
\sup_{s \in \mathcal{F}, t \in \mathcal{G}} \text{Cov}(s(X), (f^*(X) - h(X) + \varepsilon)) \geq \lim_{n \to \infty} \text{Cov}(s_n(X), f^*(X) - h(X) + \varepsilon)
\]

\[
\geq \text{Cov}(f^*(X) - h(X)) = \text{Var}(f^*(X) - h(X))
\]

Recalling the bias-variance decomposition:

\[
\mathbb{E} \left[(Y - h(X))^2\right] = \text{Var}(f^*(X) - h(X)) + (\mathbb{E}[f^*(X) - h(X)])^2 + \mathbb{E}[\varepsilon^2],
\]

we now see that the HSIC-loss minimizes the variance part of the mean squared error (MSE). To minimize the entire MSE, the learned function should be adjusted with an estimated bias.

4.1.1 The realizable case

If \( h \in \mathcal{H} \) has HSIC-loss equal to zero, then up to a constant term, it is the correct function:
Corollary 4. Under the assumptions of Theorem 2 we have the following:
\[ \text{HSIC} \left( X, Y - h(X); \tilde{F}, \tilde{G} \right) = 0 \Rightarrow h(X) = f^*(X) + c, \]
after almost everywhere.

Proof. From Theorem 2 we have that
\[ \text{HSIC} \left( X, Y - h(X); \tilde{F}, \tilde{G} \right) = 0 \iff \text{Var} \left( f^*(X) - h(X) \right) = 0, \]
therefore \( f^*(X) - h(X) \) must be a constant up to a zero-probability set of \( X \).

4.2 Robustness against covariate shift

Due to its formulation as a supremum over a large set of functions, the HSIC-loss is an upper bound to the amount by which any loss function \( \ell \) can increase due to a change in the marginal distribution of \( X \). This notion, which will be formalised in the following lemma, captures that amount by which the performance of a model might change as a result of covariate shift, where the performance is any that can be measured by some loss functions acting on the residuals.

We denote by \( D_{\text{source}} \) the density function of the distribution on \( X \) from which the training samples are drawn, and \( D_{\text{target}} \) the density of an unknown target distribution over \( \mathcal{X} \).

Theorem 5. Let \( Q \) denote the set of density functions on \( \mathcal{X} \) which are absolutely continuous w.r.t. \( D_{\text{source}} \), and their density ratio is in \( \mathcal{F} \):
\[
Q = \left\{ D_{\text{target}} : \mathcal{X} \to \mathbb{R}_{\geq 0} \quad \text{s.t.} \quad \mathbb{E}_{x \sim D_{\text{target}}} [1] = 1, \mathbb{E}_{x \sim D_{\text{source}}} \left[ \frac{D_{\text{target}}(x)}{D_{\text{source}}(x)} \right] = 1, \frac{D_{\text{target}}}{D_{\text{source}}} \in \mathcal{F} \right\}.
\]

Then,
\[
\sup_{D_{\text{target}} \in Q} \mathbb{E}_{x \sim D_{\text{source}}} [\ell(Y - h(X))] \leq M_F \cdot M_G \cdot \text{HSIC}(X, Y - h(X); \tilde{F}, \tilde{G}),
\]
where HSIC is of course evaluated on the training distribution \( D_{\text{source}} \).

Proof. We have:
\[
\text{HSIC}(X, Y - h(X); \tilde{F}, \tilde{G}) \geq \sup_{s \in \tilde{F}, t \in \tilde{G}} \left( \mathbb{E}_{x \sim D} [s(X)\ell(Y - h(X))] - \mathbb{E}_{x \sim D_{\text{source}}} [s(X)] \mathbb{E}_{x \sim D_{\text{source}}} [\ell(Y - h(X))] \right)
\]
\[
= \frac{1}{M_F \cdot M_G} \sup_{s \in \tilde{F}, t \in \tilde{G}} \left( \mathbb{E}_{x \sim D_{\text{source}}} [s(X)\ell(Y - h(X))] - \mathbb{E}_{x \sim D_{\text{source}}} [s(X)] \mathbb{E}_{x \sim D_{\text{source}}} [\ell(Y - h(X))] \right)
\]
\[
\geq \frac{1}{M_F \cdot M_G} \sup_{s \in \tilde{F}, t \in \tilde{G}} \left( \mathbb{E}_{x \sim D_{\text{source}}} [s(X)\ell(Y - h(X))] - \mathbb{E}_{x \sim D_{\text{source}}} [s(X)] \mathbb{E}_{x \sim D_{\text{source}}} [\ell(Y - h(X))] \right)
\]
\[
= \frac{1}{M_F \cdot M_G} \mathbb{E}_{x \sim D_{\text{target}}} [\ell(Y - h(X))] - \mathbb{E}_{x \sim D_{\text{source}}} [\ell(Y - h(X))].
\]

The first equality is an immediate result of 2 and the identity \( \text{Cov}(A, B) = \mathbb{E}[AB] - \mathbb{E}[A] \mathbb{E}[B] \). The second inequality is by the restriction from \( \mathcal{F} \) to \( \mathcal{S} \). The final equality is by the assumption that for all \( D_{\text{target}} \in Q, \mathbb{E}_{x \sim D} \left[ \frac{D_{\text{target}}}{D_{\text{source}}}(x) \right] = 1 \), i.e. that \( D_{\text{target}} \) is absolutely continuous with respect to \( D \).

Theorem 5 shows that the HSIC-loss is an upper bound to the amount by which any loss function \( \ell \in \mathcal{G} \) can increase due to a change in the marginal distribution of \( X \). The upper bounds holds as long as the density ratio of the (unknown) target distribution is absolutely continuous w.r.t. the source distribution \( D_{\text{source}} \) and as long as their density ratio \( \frac{D_{\text{target}}}{D_{\text{source}}} \) lies in the function space \( \mathcal{F} \). The functions \( \ell \in \mathcal{G} \) can be any loss function of the residuals, say some \( l_p \) loss, as long as they lie in \( \mathcal{G} \) or its closure.

Finally, we note that this upper bound holds without assuming that \( \mathcal{H} \) is well-specified.

Combining Theorem 5 and the lower bound of Theorem 4 we obtain the following result:
Corollary 6. Under the same assumptions of Theorems 3 and 5 further assume that the square function \( x \mapsto x^2 \), belongs to \( \mathcal{G} \) or its closure. Denote: 
\[
\delta_{\text{HSIC}}(h) = \text{HSIC}(X,Y - h(X); \mathcal{F}, \mathcal{G}),
\]
then:
\[
\text{MSE}_{\text{target}}(h) = E_{\mathcal{D}_{\text{target}}}[(Y - h(X))^2], \quad \text{bias}_{\text{source}}(h) = E_{\mathcal{D}_{\text{source}}}[f^*(x) - h(x)], \quad \text{and } \sigma^2 = E[\varepsilon^2].
\]
Then:
\[
\sup_{\mathcal{D}_{\text{target}} \in \mathcal{Q}} \text{MSE}_{\text{target}}(h) \leq 2M_F \cdot M_G \cdot \delta_{\text{HSIC}}(h) + \text{bias}_{\text{source}}(h)^2 + \sigma^2.
\]

Proof. By the lower bound of Theorem 3 we get \( \text{Var}(f^*(X) - h(X)) \leq M_F \cdot M_G \cdot \delta_{\text{HSIC}} \). By Theorem 5 and the assumption we get that:
\[
M_F \cdot M_G \cdot \delta_{\text{HSIC}}(h) \geq \sup_{\mathcal{D}_{\text{target}} \in \mathcal{Q}} \text{E}_{\mathcal{D}_{\text{target}}}[E_{\mathcal{D}_{\text{source}}}[f^*(X) + \varepsilon] - h(X)^2]
\]
\[
= \sup_{\mathcal{D}_{\text{target}} \in \mathcal{Q}} \left( \text{E}_{\mathcal{D}_{\text{target}}}[E_{\mathcal{D}_{\text{source}}}[f^*(X) + \varepsilon] - h(X) - (\text{E}_{\mathcal{D}_{\text{source}}}[f^*(X) - h(X)])^2 - E[\varepsilon^2] \right)
\]
\[
= \sup_{\mathcal{D}_{\text{target}} \in \mathcal{Q}} \left( \text{MSE}_{\text{target}}(h) - \text{Var}[f^*(X) - h(X)] - \text{bias}_{\text{source}}(h)^2 - \sigma^2 \right).
\]
Together, these inequalities give the result. \( \square \)

What Corollary 6 means is that the squared-loss in an unsupervised covariate shift scenario is bounded by terms dependent on the HSIC-loss, the source bias squared, and the inherent noise level of the problem. Assuming \( \varepsilon \) has zero mean, \( \text{E}_{\mathcal{D}_{\text{source}}}[f^*(X)] \) can be easily estimated, and thus the bias term in the error can be eliminated as HSIC is invariant to adding constants.

4.3 Learnability

So far we have obtained results showing that the HSIC-loss is related to natural measures of performance and robustness for any given hypothesis \( h \). However, an important prerequisite to using it as a loss function is the learnability question: Does \( \min_{h \in \mathcal{H}} \text{HSIC} \) converge to \( \min_{h \in \mathcal{H}} \text{HSIC} \)? We prove that under standard assumptions, HSIC is learnable in a uniform convergence sense – its empirical estimate converges to the population uniformly over all the functions in the hypothesis class.

Let us first recall the definition of the Rademacher complexity of a function class.

Definition 7. Let \( \mathcal{D} \) be a distribution over \( \mathcal{Z} \), and let \( S = \{ z_i \}_{i=1}^n \) be \( n \) i.i.d. samples. The empirical Rademacher complexity of a function class \( \mathcal{F} \) is defined as:
\[
\mathcal{R}_n(\mathcal{F}) = \mathcal{E}_{\pi} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \sigma_i h(z_i) \right].
\]

Using standard learning theory results (Mohri et al. [14], Ch 3), we prove that it is possible to minimize the HSIC objective on hypothesis classes with bounded Rademacher complexity.

Theorem 8. Suppose the residuals' kernel \( k \) is bounded in \([0, 1]\) and satisfies the following condition: \( k(r, r') = \ell(h(x) - h(x'), y - y') \) where \( \ell: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \) is s.t. \( \ell(\cdot, \cdot) \) is an \( L_\ell \)-Lipschitz function for all \( y \). Let \( C_1 = \sup_{x, x'} \ell(x, x') \), \( C_2 = \sup_{r, r'} k(r, r') \). Then, with probability of at least \( 1 - \delta \), the following holds for all \( h \in \mathcal{H} \):
\[
\left| \text{HSIC}(X, Y - h(X); \mathcal{F}, \mathcal{G}) - \text{HSIC}(\{(x_i, r_i)\}_{i=1}^n; \mathcal{F}, \mathcal{G}) \right| \leq \frac{3C_1}{n} \left( 4L_\ell \mathcal{R}_n(\mathcal{H}) + O \left( \sqrt{\frac{\ln(1/\delta)}{n}} \right) \right) + 3C_2 C_1 \sqrt{\frac{\ln(2/\delta)}{2n}}.
\]

Proof. The proof can be found in the appendix. \( \square \)
5 Related work

As mentioned above, Mooij et al. [15] were the first to propose using the HSIC loss as a means to learn a regression model. However, their work focused exclusively on learning the functions corresponding to edges in a causal graph, and leveraging that to learn causal directions and then the structure of the graph itself. They have not applied the method to domain adaptation or to robust learning, nor did they analyze the qualities of this objective as a loss function.

The literature on robust learning is rapidly growing in size and we cannot hope to cover it all here. Especially relevant papers on robust learning for unsupervised domain adaptation are Namkoong and Duchi [16], Volpi et al. [28], Duchi and Namkoong [4]. Volpi et al. [28] propose an iterative process whereby the training set is augmented with adversarial examples that are close in some feature space, to obtain a perturbation of the distribution. Namkoong and Duchi [16] suggest minimizing the variance of the loss in addition to its empirical mean, and employ techniques from learning distributionally robust models. Some recent papers have highlighted strong connections between causal inference and robust learning, see e.g. the works of Heinze-Deml and Meinshausen [10] and Rothenhäusler et al. [19]. By having some knowledge on the corresponding data generating graph of the problem, Heinze-Deml and Meinshausen [10] propose minimizing the variance under properties that are presupposed to have no impact on the prediction. A more general means of using the causal graph to learn robust models is given by Subbaswamy and Saria [24], Subbaswamy et al. [25], who propose a novel graph surgery estimator which specifically takes account of factors in the data which are known apriori to be vulnerable to changes in the distribution. These methods require detailed knowledge of the causal graph and are computationally heavy when the dimension of the problem grows. In [19], the authors propose using anchors, which are covariates that are known to be exogenous to the prediction problem, to obtain robustness against distribution shifts induced by the anchors. Of course, a large body of work exist on covariate shift learning when there is access to unlabeled test data (see, e.g., Daume and Marcu [3], Saenko et al. [20], Gretton et al. [9], Tzeng et al. [20], Volpi et al. [27]), however we stress that we do not require such access.

6 Experimental results

To evaluate the performance of the HSIC loss function, we experiment with synthetic and real-world data. We focus on tasks of unsupervised transfer learning: we train on a one distribution, called the SOURCE distribution, and test on a different distribution, called the TARGET distribution. We assume we have no samples from the target distribution during learning.

6.1 Synthetic data

As a first evaluation of the HSIC-loss, we experiment with fitting a linear model. We focus on small sample sizes as those often lead to difficulties in covariate shift scenarios. The underlying model in the experiments is \( y = \beta^T x + \epsilon \) where \( \beta \in \mathbb{R}^{100} \) is drawn for each experiment from a Gaussian distribution with \( \sigma = 0.1 \). In the training phase, \( x \) is drawn from a uniform distribution over \([-1, 1]^{100}\). We experimented with \( \epsilon \) drawn from one of three distributions: Gaussian, Laplacian, or a shifted exponential: \( \epsilon = 1 - e \) where \( e \) is drawn from an exponential distribution \( \exp(1) \). In any case, \( \epsilon \) is drawn independently from \( x \). In each experiment, we draw \( n \in \{2^i\}_{i=5}^{13} \) training samples and train using either using squared-loss, absolute-loss, and HSIC-loss, all with an \( l_2 \) regularization term. In order to find the \( l_2 \) regularization parameter, we perform cross validation on validation data created from 10% of the training set, where the possible values are in \{15, 12, 10, 5, 1, 0.1, 0.01, 0.001, 0.0001, 0, 0.00001\}, for absolute- and HSIC-losses, and \{35, 37, ..., 69\} for the squared-loss. The model is then trained on all of the training data, and is evaluated on two test sets each of size \( 100 \cdot n \). The SOURCE test set is created in the same manner as the training set was created, while the TARGET test set simulates a covariate shift scenario. This is done by changing the marginal distribution of \( x \) from a uniform distribution to a Gaussian distribution over \( \mathbb{R}^{100} \). In all cases the noise on the SOURCE and TARGET is drawn from the same distribution. This process is repeated 20 times for each \( n \). When training the models with HSIC-loss, we used batch-size of 32, and optimized using Adam optimizer [11], with learning rate drawn from a uniform distribution over \([0.0001, 0.0002]\). The kernels we chose were radial basis function kernels, with \( \gamma = 1 \) for both covariates' and residuals' kernels. When training with absolute-loss, we used stochastic gradient descent, with initial learning rate determined by cross validation.
Figure 1: Comparison of models trained with squared-loss, absolute-loss and HSIC-loss. Each point on the graph is the MSE averaged over 20 experiments, and the shaded area represents one standard error from the mean. Dashed lines are the MSE evaluated over the source distribution, solid lines are the MSE evaluated over the target distribution.

from \{0.05, 0.01, 0.005, 0.001, 0.0005, 0.00005, 0.000001\}, and later decayed using inverse scaling.

Figure 1 presents the results of experiments with Gaussian, Laplacian, and shifted-exponential noise. With Gaussian noise, HSIC-loss performs similarly to squared-loss regression, and with Laplacian noise HSIC-loss performs similarly to absolute-loss regression, where squared-loss is the maximum-likelihood objective for Gaussian noise and absolute-loss is the maximum-likelihood objective for Laplacian noise. In both cases it is reassuring to see that HSIC-loss is on par with the maximum-likelihood objectives. In all cases we see that HSIC-loss is better on the TARGET distribution compared to objectives which are not the maximum likelihood objective. This is true especially in small sample sizes. We believe this reinforces our result in Theorem 5 that the HSIC-loss is useful when we do not know in advance the loss or the exact target distribution.

6.2 Bike sharing dataset

In the bike sharing dataset by Fanaee-T and Gama [5] from the UCI repository, the task is to predict the number of hourly bike rentals based on the following covariates: temperature, feeling temperature, wind speed and humidity. Consisting of 17,379 samples, the data was collected over two years, and can be partitioned by year and season. This dataset has been used to examine domain adaptation tasks by Subbaswamy et al. [25] and Rothenhäusler et al. [19]. We adopt their setup, where the SOURCE distribution used for training is three seasons of a year, and the TARGET distribution used for testing is the forth season of the same year, and where the model of choice is linear. We compare with least squares, anchor regression (AR) Rothenhäusler et al. [19] and Surgery by Subbaswamy et al. [25].

We ran 100 experiments, each of them was done by randomly sub-sampling 80% of the SOURCE set and 80% of the TARGET set, thus obtaining a standard error estimate of the mean. When training the models with HSIC-loss, we used batch-size of 32, and optimized the loss with Adam [11], with learning rate drawn from a uniform distribution over [0.0008, 0.001]. The kernels we chose were radial basis function kernels, with $\gamma = 2$ for the covariates’ kernel, and $\gamma = 1$ for the residuals’ kernel.

We present the results in Table 1. Following the discussion in section 4, we report the variance part of the MSE on the test set. We can see that training with HSIC-loss results in better performances in 6 out of 8 times. In addition, unlike AR and Surgery, training with HSIC-loss does not require knowledge of the specific causal graph of the problem, nor does it require the training to be gathered from different sources as in AR.
Table 1: Variance results on the bike sharing dataset. Each row corresponds to a training set consisting of three season of that year, and the variance of $Y - h(X)$ the \texttt{TARGET} set consisting of the forth season. In bold are the best results in each experiment, taking into account one standard error.

| Test data OLS | AR | Surgery | HSIC |
|--------------|----|---------|------|
| $(Y1)$ Season 1 | 15.4±0.02 | 15.4±0.02 | 15.5±0.03 | 16.0±0.04 |
| Season 2 | 23.1±0.03 | 23.2±0.03 | 23.7±0.04 | 22.9±0.03 |
| Season 3 | 28.0±0.03 | 28.0±0.03 | 28.1±0.03 | 27.9±0.03 |
| Season 4 | 23.7±0.03 | 23.7±0.03 | 25.6±0.04 | 23.6±0.04 |
| $(Y2)$ Season 1 | 29.8±0.05 | 29.8±0.05 | 30.7±0.06 | 30.7±0.07 |
| Season 2 | 39.0±0.05 | 39.1±0.05 | 39.2±0.06 | 38.9±0.04 |
| Season 3 | 41.7±0.05 | 41.5±0.05 | 41.8±0.05 | 40.8±0.05 |
| Season 4 | 38.7±0.04 | 38.6±0.04 | 40.3±0.06 | 38.6±0.05 |

6.3 Rotating MNIST

In this experiment we test the performance of models trained on the MNIST dataset by LeCun et al. \cite{12} as the \texttt{SOURCE} distribution, and digits which are rotated by an angle $\theta$ sampled from a uniform distribution over $[-45, 45]$ as the \texttt{TARGET} distribution. Figure 3 shows samples of the test data. The standard approach to obtain robustness against such perturbations is to augment the training data with images with similar transformations, as in Schölkopf et al. \cite{21} for example. However, in practice it is not always possible to know in advance what kind of perturbations should be expected, and therefore it is valuable to develop methods for learning robust models even without such augmentations. We compared training with HSIC-loss to training with cross entropy loss, using three types of architectures. The first is a convolutional neural network (CNN): $\texttt{input} \rightarrow \texttt{conv(dim=32)} \rightarrow \texttt{conv(dim=64)} \rightarrow \texttt{fully-connected(dim=524)} \rightarrow \texttt{dropout(p=0.5)} \rightarrow \texttt{fully-connected(dim=10)}$. The second is a multi-layered perceptron (MLP) with two hidden layers of size 256, 524, 1024: $\texttt{input} \rightarrow \texttt{fully-connected(dim=256)} \rightarrow \texttt{fully-connected(dim=524)} \rightarrow \texttt{dropout(p=0.5)} \rightarrow \texttt{fully-connected(dim=10)}$. The third architecture was also an MLP, except there were four hidden layers instead of two. Each experiment was repeated 20 times, and in every experiment the number of training steps (7 epochs) remained constant for a fair comparison. Each time the training set consisted of 10K randomly chosen samples. Both losses were optimized using Adam \cite{11}, and the learning rate was drawn each
time from a uniform distribution over $[10^{-4}, 4 \cdot 10^{-4}]$. Experimenting with different regimes of the learning rate gave similar results. The kernels we chose were radial basis function kernels with $\gamma = 1$ for the residuals, and $\gamma = 22$ for the images, chosen according to the heuristics suggested by Mooij et al. [15]. The results are depicted in Figure 2. We see that for all models, moving to the TARGET distribution induces a large drop in accuracy. Yet for all architectures we see that using HSIC-loss gives better performance on the TARGET set compared to using the standard cross-entropy loss.

7 Conclusion

In this paper we propose learning models whose errors are independent of their inputs, as way to defend against worst-case covariate shift scenarios. This can be view as a non-parametric generalization of the way residuals are orthogonal to the instances in OLS regression. We prove that the HSIC-loss is learnable in terms of uniform convergence, and show that learning with this loss is robust against changes in the input distribution as long as the density ratio function is within a bounded RKHS. In experiments, we showed that learning with the HSIC-loss achieves performance which is comparable to standard loss functions on the source distribution, but is significantly better on the target distribution in the case when one has no access to target samples during training. An interesting future direction is to better understand the connection between this type of loss, originally proposed in the context of learning causal graph structure, and the idea of learning causal models that are expected to be robust against distributional changes [13][2].

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We then show how we can treat this as a learning problem over pairs of instances, where the objective
is to predict the difference in \( y \), allowing us to use standard tools and concentration bounds.

Recall that the empirical estimation problem we pose is

\[
\sup_{h \in \mathcal{H}} \left| E_{r,r'} [k (r,r')] - \frac{1}{(n)_2} \sum_{i=2}^{n} k (r_{i1}, r_{i2}) \right|.
\]

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\]

We then show how we can treat this as a learning problem over pairs of instances, where the objective
is to predict the difference in \( y \), allowing us to use standard tools and concentration bounds.
Using simple algebra, one can obtain the following bound for (6):

\[
\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,x',r,r'} \left[ k(r,r') l(x,x') \right] - \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) l(x_{i1},x_{i2}) \right|
\]

\[
= \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,x',r,r'} \left[ k(r,r') l(x,x') \right] - \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) l(x_{i1},x_{i2}) \right|
+ \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) \mathbb{E} [l(x,x')] \left( l(x_{i1},x_{i2}) \right)
\]

\[
\leq \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,x',r,r'} \left[ k(r,r') l(x,x') \right] - \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) l(x_{i1},x_{i2}) \right|
+ \sup_{h \in \mathcal{H}} \left| \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) \left( l(x_{i1},x_{i2}) \right) - l(x_{i1},x_{i2}) \right|
\]

\[
\leq C_1 \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,x',r,r'} \left[ k(r,r') l(x,x') \right] - \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) \right|
+ C_2 \sup_{h \in \mathcal{H}} \left| \mathbb{E} [l(x,x')] - \frac{1}{(n)^2} \sum_{i,j} l(x_{i1},x_{i2}) \right|
\]

\[
= C_1 \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{r,r'} \left[ k(r,r') \right] - \frac{1}{(n)^2} \sum_{i,j} k(r_{i1},r_{i2}) \right|
+ C_2 \mathbb{E} [l(x,x')] - \frac{1}{(n)^2} \sum_{i,j} l(x_{i1},x_{i2})
\]

Where the first inequality follows from properties of \(\sup\), the second inequality follows from the definitions of \(C_1\) and \(C_2\), and the last equality follows from the fact that the second term does not
depend on $h$. Similarly, (7) can be bounded as follows:

\[
\sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ \mathbb{E}_{x'} \left[ I (x, x') \right] \mathbb{E}_{r'} \left[ k (r, r') \right] \right] \right|
\]

\[
- \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) I (x_{i_2}, x_{i_3})
\]

\[
= \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ \mathbb{E}_{x'} \left[ I (x, x') \right] \mathbb{E}_{r'} \left[ k (r, r') \right] \right] \right|
\]

\[
- \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) I (x_{i_2}, x_{i_3})
\]

\[
+ \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) \mathbb{E}_{x,x'} \left[ I (x, x') \right]
\]

\[
- \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) \mathbb{E}_{x,x'} \left[ I (x, x') \right]
\]

\[
= \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ \mathbb{E}_{x'} \left[ I (x, x') \right] \mathbb{E}_{r'} \left[ k (r, r') \right] \right] \right|
\]

\[
- \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) \mathbb{E}_{x,x'} \left[ I (x, x') \right]
\]

\[
+ \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) \left( \mathbb{E}_{x,x'} \left[ I (x, x') \right] - I (x_{i_2}, x_{i_3}) \right)
\]

\[
\leq \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ \frac{1}{(n)_3} \sum_{i \in [3]} \left( \mathbb{E}_{x'} \left[ k (r, r') \right] \right. \right.
\]

\[
- k (r_{i_1}, r_{i_2}) \left. \mathbb{E}_{x'} \left[ I (x, x') \right] \right) \mathbb{E}_{x,x'} \left[ I (x, x') \right]
\]

\[
+ \sup_{h \in \mathcal{H}} \left| \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2}) \left( \mathbb{E}_{x,x'} \left[ I (x, x') \right] - I (x_{i_2}, x_{i_3}) \right) \right|
\]

\[
\leq \sup_{x} \mathbb{E}_{x'} \left[ I (x, x') \right] \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ \mathbb{E}_{x'} \left[ k (r, r') \right] \right] \right|
\]

\[
- \frac{1}{(n)_3} \sum_{i \in [3]} k (r_{i_1}, r_{i_2})
\]

\[
+ \sup_{r, r'} \left| \mathbb{E}_{x,x'} \left[ I (x, x') \right] - \frac{1}{(n)_3} \sum_{i \in [3]} I (x_{i_2}, x_{i_3}) \right|
\]

\[
\leq C_{1} \sup_{h \in \mathcal{H}} \left| \mathbb{E}_{x,r} \left[ k (r, r') \right] \right| - \frac{1}{(n)_2} \sum_{i \in [2]} k (r_{i_1}, r_{i_2})
\]

\[
+ C_{2} \left| \mathbb{E}_{x,x'} \left[ I (x, x') \right] - \frac{1}{(n)_2} \sum_{i \in [2]} I (x_{i_1}, x_{i_2}) \right|,
\]
where the first inequality follows from properties of \( \sup \), and the last inequality follows from the definition of \( C_1 \) and \( C_2 \), and the definitions of \( (n)_m \). And finally, the same reasoning can be applied to bound \( [8] \):

\[
\begin{align*}
\sup_{h \in \mathcal{H}} & \left| \mathbb{E}_{r,r'} \left[ k \left( r, r' \right) \right] \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] \right| \\
- \frac{1}{(n)_4} \sum_{i \leq 4} k \left( r_{i1}, r_{i2} \right) l \left( x_{i3}, x_{i4} \right) & = \mathbb{E}_{r,r'} \left[ k \left( r, r' \right) \right] \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] \\
& - \frac{1}{(n)_4} \sum_{i \leq 4} k \left( r_{i1}, r_{i2} \right) l \left( x_{i3}, x_{i4} \right) \\
& + \frac{1}{(n)_4} \sum_{i \leq 4} k \left( r_{i1}, r_{i2} \right) \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] \\
& \leq \mathbb{E}_{r,r'} \left[ k \left( r, r' \right) \right] - \frac{1}{(n)_4} \sum_{i \leq 4} k \left( r_{i1}, r_{i2} \right) \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] \\
& + \frac{1}{(n)_4} \sum_{i \leq 4} k \left( r_{i1}, r_{i2} \right) \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] - l \left( x_{i3}, x_{i4} \right) \\
& \leq C_1 \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] - \frac{1}{(n)_2} \sum_{i \leq 2} l \left( x_{i1}, x_{i2} \right) + C_2 \mathbb{E}_{x,x'} \left[ l \left( x, x' \right) \right] - \frac{1}{(n)_2} \sum_{i \leq 2} l \left( x_{i1}, x_{i2} \right). 
\end{align*}
\]

Now, the second term of the RHS of the bound in Lemma 9 can be bounded using standard techniques such as Hoeffding’s inequality. We therefore shift our attention to the first term. This term can be bounded using Rademacher based techniques.

First, we assume that \( k \left( r, r' \right) = s \left( r - r' \right) \) for some function \( s \) with Lipschitz constant \( L_s \). Next, we define a distribution over \( \mathcal{X} \times \mathcal{X} \times \mathcal{Y} \) by \( p' \left( \mathbf{x} \right) = p' \left( \left( x, x' \right) \right) = p \left( x \right) p \left( x' \right) \), and we let \( y \left( x, x', \varepsilon, \varepsilon' \right) = f \left( x \right) - f \left( x' \right) + \varepsilon - \varepsilon' \). Now, we can define a new function class

\[
\mathcal{H}^2 = \left\{ \left( x_1, x_2 \right) \mapsto h \left( x_1 \right) - h \left( x_2 \right) \mid h \in \mathcal{H} \right\},
\]

and consider

\[
\sup_{h \in \mathcal{H}^2} \left| \mathbb{E}_{x,y} \ell \left( h \left( x \right), y \right) - \sum_{i=1}^{n} \ell \left( h \left( x_i \right), y_i \right) \right|
\]

where \( \ell \left( h \left( x \right), y \right) = s \left( r_1 - r_2 \right) \). This is exactly the first term in the bound, which can be bounded using standard generalization bounds. The only missing pieces left are how to relate the Rademacher complexity of \( \mathcal{H}^2 \) to that of \( \mathcal{H} \), and how the Lipschitz constant of the residuals’ kernel affects it.

**Lemma 10.** \( \mathcal{R}_{n} \left( \mathcal{H}^2 \right) \leq 2 \mathcal{R}_{n} \left( \mathcal{H} \right) \).
where the first inequality is due to the fact that $1 + \gamma M > 1$ for some $\gamma > 0$.

As for the Lipschitz constant, a known result relating the Rademacher complexity of a function class to the uniform convergence result based on the Rademacher complexity of a class is the following.

**Theorem 11** (Sham Kakade [23]). Let $\ell : \mathbb{R} \times \mathcal{Y} \to \mathbb{R}$ be s.t. $\ell(\cdot, y)$ is an $L$-Lipschitz function for all $y$. Denote $\ell \circ \mathcal{H} = \{(x, y) \mapsto \ell(h(x), y) \mid h \in \mathcal{H}\}$. Then,

$$\mathcal{R}_n(\ell \circ \mathcal{H}) \leq L \cdot \mathcal{R}_n(\mathcal{H}).$$

As an example, the following lemma proves the Lipschitz condition for RBF kernels.

**Lemma 12.** Assume $\ell(z, y) = \exp(-\gamma(z - y)^2)$, as is the case with RBF kernels, and suppose $|y| \leq \frac{M}{2}$ for some $M > 0$ for all $y$. Then $\ell(\cdot, y)$ is $M$-Lipschitz for all $y$.

**Proof.** Let $\ell(z, y) = \exp(-\gamma \|z - y\|^2)$ for some $\gamma > 0$, and suppose $\|y\| \leq \frac{M}{2}$ for some $M > 0$ for all $y \in \mathcal{Y}$. Then,

$$\exp(-\gamma \|y - z_1\|^2) - \exp(-\gamma \|y - z_2\|^2) \leq \gamma (\|y - z_1\|^2 - \|y - z_2\|^2) \leq \gamma \cdot M \|z_1 - z_2\|^2,$$

where the first inequality is due to the fact that $1 + x \leq e^x$, the second is due to the fact that $\exp(-c) \leq 1 \forall c \geq 0$, the third is due to triangle inequality and the last is due to the definition of $M$.

Before concluding, we state the uniform convergence result based on the Rademacher complexity of a class.

**Theorem 13** (Mohri et al. [14], Ch. 3). Suppose $f(z) \in [0, 1]$ for all $f \in \mathcal{F}$, and let $\delta \in (0, 1)$. Then, with probability of at least $1 - \delta$ over the choice of $S$, the following holds uniformly for all $f \in \mathcal{F}$:

$$\left| \mathbb{E}_D[f(z)] - \frac{1}{n} \sum_{i=1}^{n} f(z_i) \right| \leq 2 \mathcal{R}_n(\mathcal{F}) + O\left(\sqrt{\frac{\ln(1/\delta)}{n}}\right).$$

Equipped with those results, the learnability Theorem immediately follows.

**Proof of Theorem.** This is a direct application of the previous lemmas and Hoeffding’s inequality.